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SAFEPAQ-II: User manual

R.A. Forrest

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EURATOM/UKAEA Fusion Association

Culham Science Centre
Abingdon
Oxfordshire
OX14 3DB
United Kingdom

Telephone: +44 1235 466586
Facsimile: +44 1235 466435

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SAFEPAQ-II: User manual

R. A. Forrest

EURATOM/UKAEA Fusion Association, Culham Science Centre,
Abingdon, Oxfordshire OX14 3DB, UK

Abstract

SAFEPAQ-II is the software tool that has been developed to enable efficient production of the EAF nuclear data libraries that are required as input to the FISPACT activation code. It forms part of the European Activation System (EASY), and replaces SAFEPAQ and SYMPAL that were used previously.

SAFEPAQ-II enables all the nuclear data to be stored in relational databases (Access) and by using an interactive user interface allows the data to be viewed, modified, validated and then produced in the required EAF format as text files. It is written in Visual Basic and runs under the Windows NT4, 98, 2000 and XP operating systems. The Windows operating system has the great advantage of portability and SAFEPAQ-II has been successfully installed at two external sites for use by UKAEA's international collaborators. It has been used in the production of the EAF-2001, EAF-2003, EAF-2005 and EAF-2007 data libraries.

Significant changes and enhancements have been made to SAFEPAQ-II for the production of the EAF-2007 data libraries. An important reason for the changes is the need to be able to treat data for deuteron- and proton-induced reactions with an upper energy of 60 MeV. The method of Statistical Analysis of Cross Sections (SACS) is a major new feature added for the present issue.

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Introduction

The European Activation System (EASY) is the complete package of data, inventory code and processing system for activation calculations that is maintained by the Euratom/UKAEA Fusion Association at Culham Science Centre. Maintenance of the EAF nuclear data libraries is a complex procedure; the cross section files need to be evaluated (including choosing from several sources and adjustment of data), processed (conversion to a common format), compiled into a library, validated (against experimental data and systematics) and documented. Similarly, the decay data files need to be compiled and documented, and all the subsidiary files required as input to the inventory code FISPACT [1] need to be generated in a consistent manner.

The SYMPAL processing system, which originated at ECN Petten, has been used previously to carry out the task of cross section library processing. Details of the usage of SYMPAL are covered in the User Manual [2] and the guide to the Utilities [3]. However, the tasks of evaluation and visualisation of the cross section libraries and the maintenance of the decay data library were not covered by SYMPAL. Usage of SYMPAL was complicated, and because it was not written at Culham, maintenance, improvement and quality assurance proved difficult. A first step to try and improve this was the development of the SAFEPAQ application.

SAFEPAQ (**S**ystem for **A**ctivation **F**ile **E**valuation, **P**rocessing **A**nd **Q**uality assurance) was developed and used for parts of the processing of EAF-97 and EAF-99 [4,5,6]. The user manual [7] describes the version developed in 1997. SAFEPAQ and SYMPAL were UNIX applications and the visualisation used PV-WAVE [8]. Since then many changes have occurred in the computer facilities at Culham, and it was judged necessary to reconsider the whole philosophy of nuclear data work. The main decision was to store all nuclear data in relational databases. The second was the decision to construct the User Interface to run on a Windows PC rather than under UNIX; experience with the development of such interfaces on both UNIX and PC environments had shown that the PC route was much quicker and more flexible.

The application that has been produced is named SAFEPAQ-II, it has been developed from scratch using Visual Basic; all the data are stored in Access databases and it runs under Windows XP workstation on a PC with large enough hard disks to enable all data files to be stored on-line.

Objectives

There are five main objectives of the SAFEPAQ-II application:

- Organising data
- Viewing data
- Altering data
- Processing data
- Logging modifications

Organising data

For both the cross section and decay data libraries many sources of data are required to compile the final libraries. In both cases each source library is stored in a separate folder, containing both the raw data in the native format and the Access database (for cross sections). The SAFEPAQ-II databases are stored in a separate folder that may be on a different hard disk. Although the amount of data is substantial it is possible to write all of it to DVDs which can be used to install the system on other PCs.

Viewing data

Visualisation of cross section data is a very important part of the evaluation and validation process. Data from several sources for a particular reaction can be plotted together, and to this plot can be added experimental data, either from the internal SAFEPAQ-II databases (equivalent to the 'ASCII tables' used by SYMPAL) or from the EXFOR database. As well as viewing on screen, options for printing and the production of 'books' of plots can also be selected.

The decay data can be viewed in a graphical form, including the γ- and X-ray lines of each of the radionuclides. The decay data viewer shows all decay properties such as half-life and decay modes as well as the biological hazards and other subsidiary data used by FISPACT.

Altering data

The cross section data from a particular data source usually require modification before incorporation in the final EAF library. This is handled by constructing a series of basic modifications, which are stored in a database. These can be viewed, added to and their effects tested prior to using them all to construct the final library. This modular approach of separating the data and the modifications makes checking and quality assurance very efficient.

Processing data

The basic steps of building a new EAF cross section library entail:

- Compiling all sources of data into separate databases, with details of all these sources held in the Library database.
- The selection of the data source for each reaction and the creation of the Master database containing these data.
- Improvement of the experimental data that are used in the construction of the modifications, which include branching, renormalisation, addition and merging of data. These are stored in the Parameter database.
- Apply the modifications to produce the Final database.
- Write data from Final in the standard EAF format as text files which can be used by EASY.
- In order to carry out these steps there is a need to visualise data, test the results of modifications, and compare with experiments to iterate the processes.

Logging changes

In the process of the production of a new version of the EAF library many thousands of modifications need to be made. These include use of new data sources, changes to experimental data, new nuclides, new reactions and changes to cross section data. Many iterations of visualisation, modification and processing will be required and it is essential that all permanent changes to data are automatically recorded. SAFEPAQ-II contains a comprehensive logging system that records the changes that were made. The log can be viewed and printed, and if necessary additional comments can be added. No log entries can be removed, only new ones added. The automatic logging gives a complete record and is superior to hand written records since nothing is omitted.

Getting started

This and the following sections give a 'hands-on' guide to using the application. Appendix 1 gives some design details.

When started for the first time the Settings window will open, it is essential that the user fills in the correct location of files, especially the SAFEPAQ-II databases, because the application needs to open these immediately, and an error will be caused if they are not available. Note that if this happens, i.e. that as soon as SAFEPAQ-II opens it crashes, then enter `safepaq2 /S` on the command line to enable it to start in safe mode (`/S`) so that the settings can be corrected. The option `/D` can be used to give debugging information (progress prior to a crash) in the file `C:\safepaq_debug`.

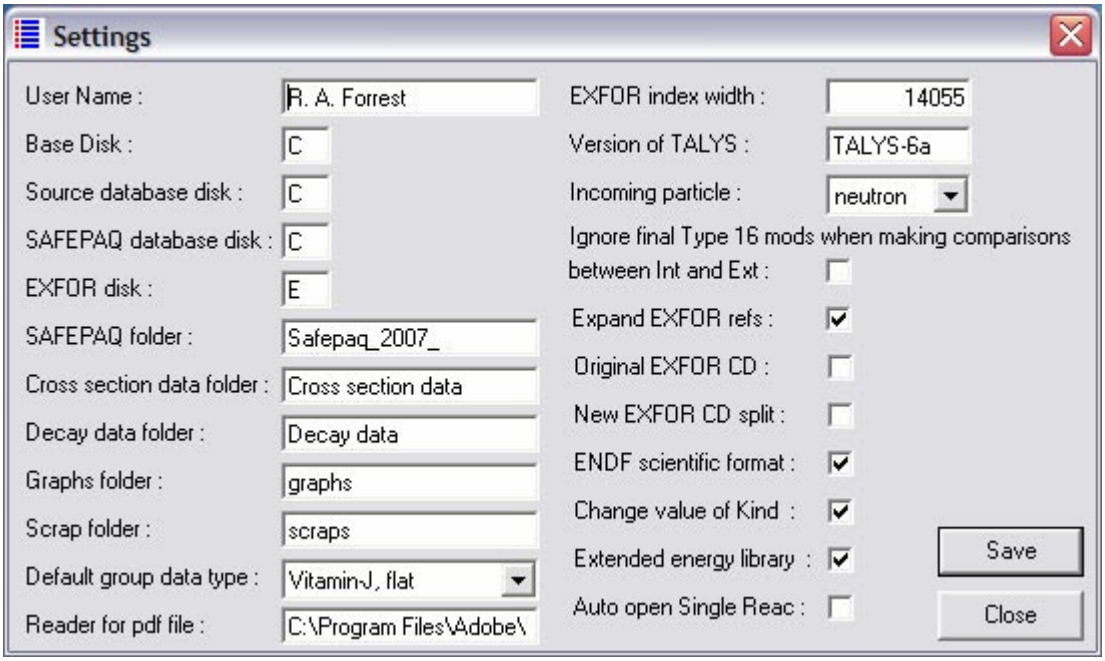


Figure 1. The Settings window.

Figure 1 shows the Settings window, the SAFEPAQ-II databases are in the `Safepaq_2007_` folder. Note that to increase flexibility, if the folder `Safepaq_2_` is detected on the Source database disk, then it is assumed that all folders (such as `Cross section data`) are in this special folder. See Appendix 2 for more details. The window can also be opened by clicking the File|Settings… menu item or the fifth toolbar button. The meaning of the various check box options are explained in the relevant section later in this report, but note here that if the project includes data at energy > 20 MeV then the Extended energy library option must be checked.

It is recommended that the supplied SAFEPAQ-II databases remain untouched, and that a new EAF project is started. Figure 2 shows the main window, note that it has menus, a toolbar (the set of buttons each with a picture) and a status bar. The name of the current EAF project is shown in the title bar.

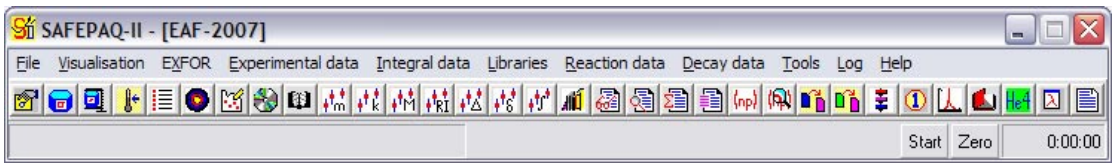

SAFEPAQ-II - [EAF-2007]
File Visualisation EXFOR Experimental data Integral data Libraries Reaction data Decay data Tools Log Help
Start
Zero
0:00:00

Figure 2. The main SAFEPAQ-II window.

The purpose of each toolbar button can be seen by resting the cursor over the button, this will display a ToolTip. Clicking on the File menu displays the File menu items, the first of these is 'New EAF project…' (this will be referred to in the text as

File|New EAF project…). Clicking this displays the New EAF project window shown in Figure 3.

Figure 3. The New EAF project window.

Enter the name and description of the new library in the first two text boxes and then click the browse button (…) to the right of the Path text box. This displays the Open dialog that enables the location of the new databases to be specified. Note that a new folder can be specified in the dialog, when this is created then just enter anything in the file name box (e.g. `dummy`) so that the path name is displayed in Figure 3. Clicking the Create button will cause the original databases to be copied to the new location, all the library specific data to be removed and the project to be renamed with the name specified in the Name text box. This process (basically file copying) takes about 2 minutes; all timings given in this report are based on a 3.2 GHz PC processing an extended energy library.

Note that from EASY-2005, projects with an upper energy limit of 20 and 60 MeV can be treated. In many cases details of menu items and windows will depend on which type is chosen; this is done by clearing or ticking the Extended energy library check box in the Settings window (Figure 1). In this report the 60 MeV library is treated as the standard, a 20 MeV library is referred to a 'non-extended library'.

Note that from EASY-2007, projects with a range of incoming particles can be created. The type of particle is determined by the Incoming particle selected in the Settings window (Figure 1). In this report most of the examples assume that this is a neutron.

Clicking the Set as current button means that SAFEPAQ-II will work with the new databases rather than the original ones. This opens the Settings window (Figure 1) with the changes displayed. Clicking the Save button implements the changes. Next the Compact databases window shown in Figure 4 is displayed. When databases are written to and then data are deleted, the storage of data can become very inefficient. To

reduce the size of the databases they need to be compacted. This window can also be displayed by clicking the File|Compact databases… menu item or the third toolbar button.

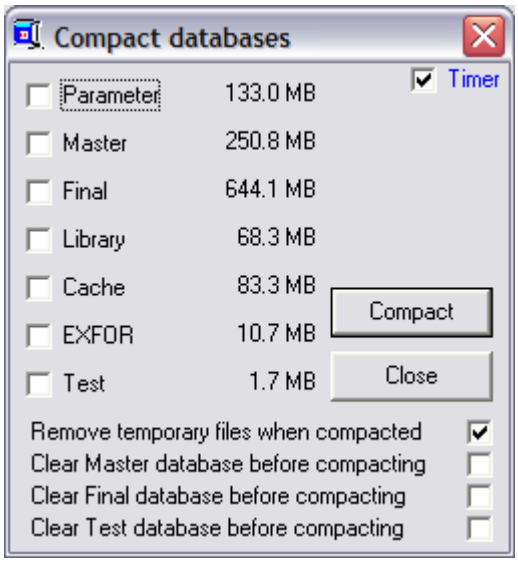


Figure 4. The Compact databases window.

Check the Parameter, Master, Final, Cache and Test options and click the Compact button. This will cause the selected databases to be compacted and the new sizes will be shown. In this case there will be a very significant reduction. At later stages of use, compacting a large database that is not empty can take significant time. Check the Timer option if you want the elapsed time to be displayed in the main window status bar. If a database is full of data that are no longer required then tick the appropriate Clear <Name> database before compacting check box to speed up the compacting. Note that the size of Final includes both *final.mdb* and (if it exists) *final_add.mdb*, see Appendix 2 for database details.

If it is required to switch to a different (existing) EAF project then this can be done by changing the location of the SAFEPAQ-II databases in the SAFEPAQ folder text box in the Settings window (Figure 1).

The status of progress towards creating a new EAF library can be monitored by displaying the Status window. This is done by clicking on File|Status… or the fourth toolbar button to display the Status window shown in Figure 5.

Note that the name of the current EAF project is given in the title bar. The Status window shows the various steps that have been completed by a red tick. On a new project there will be no ticks displayed.

It is possible that the information on the progress shown by the ticks can become incorrect due to crashes or other problems. In this case, if it is known that a step has been completed but no tick is shown, then double click on the text and the corresponding tick will be added.

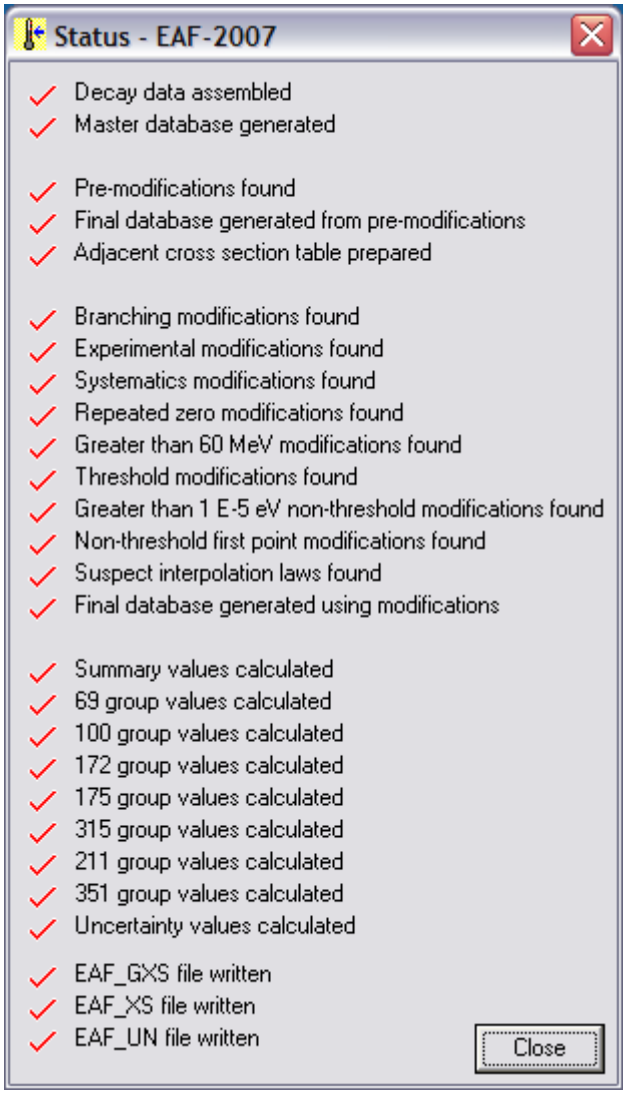


Figure 5. The Status window.

As various operations are carried out entries are made in the Log. This can be viewed by clicking on the Log|View Log… menu item or the last toolbar button to display the Log window shown in Figure 6. The date and time of the entry and the action are displayed. More entries can be seen by scrolling down. By default all entries are shown, but various classes can be displayed by clicking on the View menu and selecting a class. The available ones are: Added comments, Processing entries, Ad hoc entries, Warnings and Errors. It is possible to add a comment to an existing entry or add a new entry (which just contains a comment) by selecting items on the Edit menu. Note that shortcut keys are defined for several items, thus `Ctrl+E`

will enable a comment to be entered. The complete Log or a selected part of it can be printed out to the default printer or copied to the clipboard by clicking on the File|Print or Edit|Copy menu items respectively. Note that for QA reasons it is not possible to delete Log entries. As the Log becomes larger it is helpful to be able to search for specific entries. Clicking Edit|Find… displays the Find in Action window shown in Figure 7. Enter the string to be found in the text box and click the Find First button. The first entry containing the string (in the Action column) is shown at the top of the Log window. Subsequent entries can be found by clicking the Find Next button.

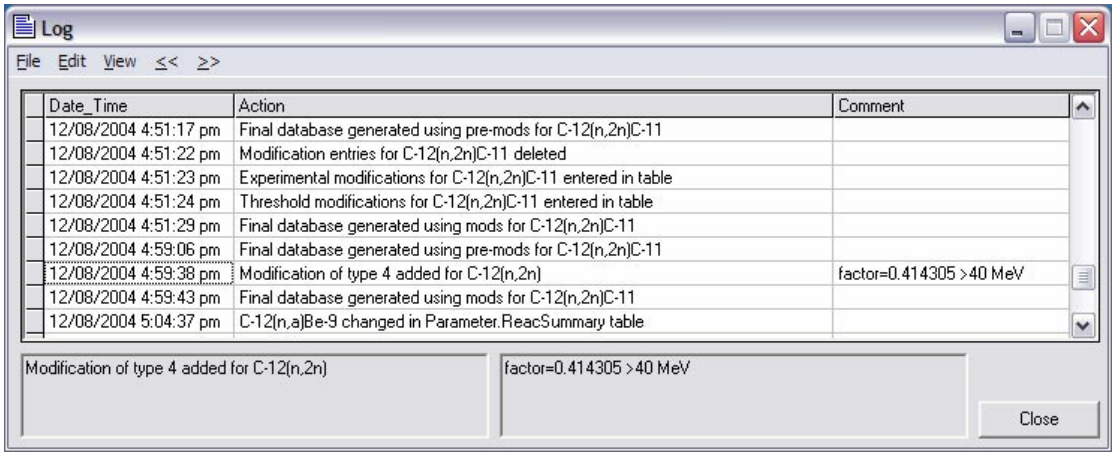

Log
File Edit View << >>
Date_Time
Action
Comment
12/08/2004 4:51:17 pm
Final database generated using pre-mods for C-12(n,2n)C-11
12/08/2004 4:51:22 pm
Modification entries for C-12(n,2n)C-11 deleted
12/08/2004 4:51:23 pm
Experimental modifications for C-12(n,2n)C-11 entered in table
12/08/2004 4:51:24 pm
Threshold modifications for C-12(n,2n)C-11 entered in table
12/08/2004 4:51:29 pm
Final database generated using mods for C-12(n,2n)C-11
12/08/2004 4:59:06 pm
Final database generated using pre-mods for C-12(n,2n)C-11
12/08/2004 4:59:38 pm
Modification of type 4 added for C-12(n,2n)
factor=0.414305 >40 MeV
12/08/2004 4:59:43 pm
Final database generated using mods for C-12(n,2n)C-11
12/08/2004 5:04:37 pm
C-12(n,a)Be-9 changed in Parameter.ReacSummary table
Modification of type 4 added for C-12(n,2n)
factor=0.414305 >40 MeV
Close

Figure 6. The Log window.

It is easy to move to the end of the Log by clicking the >> menu item, and to the start by clicking the << menu item. If the View|User ID as ToolTip option is checked then resting the cursor over the grid will give the User ID of the person who added the Log entry as a ToolTip.

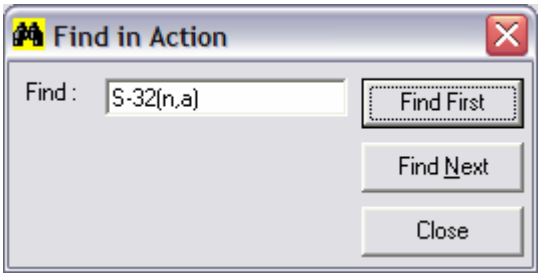


Figure 7. The Find in Action window.

The present User manual can be viewed on-line as a PDF. To do this it is necessary to have a PDF viewer on your computer. Enter the location of this in the Reader for pdf file text box in the Settings window (Figure 1). To display the User manual click the Help|View User manual menu item. Note that the User manual must be named `SAFEPAQ-II_User_manual.pdf` and must be in the `Safepaq_2_\Documents` folder.

The details of the version of SAFEPAQ-II that is being run can be found by clicking on Help|About SAFEPAQ-II to display the About SAFEPAQ-II window shown in Figure 8. This shows date, version, username, copyright and a short status report.

About SAFEPAQ-II
SAFEPAQ-II
part of
EASY-2007
SAFEPAQ-II
Version 1.0.288
21 December 2006
SAFEPAQ-II is a processing code to replace SAFEPAQ and SYMPAL, based on Access databases.
Copyright © UKAEA Fusion 2006.
R. A. Forrest
System for Activation File Processing and Quality assurance. Fully functional version. Comprehensive error trapping still to be implemented.
OK
System Info...

Figure 8. The About SAFEPAQ-II window.

Clicking on the System info… button displays the Microsoft System Information window giving a large amount of information about the system.

Printing is possible from many of the windows, such printing is to the default printer. This can be changed by clicking the File|Printer setup… menu item to display the standard Print window where a printer can be selected.

The status bar in the main window contains two buttons and a time display at the right hand side. These operate a stopwatch that can be used manually or by SAFEPAQ-II to show elapsed times of various operations. Pressing the Start button will start the timer and change the button caption to Stop. Clicking this will stop the clock. Clicking Start again will restart the timer. The timer can be reset by clicking the Zero button. Many calculations start the timer automatically, and if the last value is required to be stored for use later this can be done by clicking the File|Timer… menu item. This displays the Timer window shown in Figure 9. The current stored value and description are shown. These can be cleared by clicking the Clear button. Clicking the Overwrite button will place the current elapsed time and a description entered in the first text box in the store. Clicking the Add to button will add the current elapsed time shown on the status bar to the store and put the sum in the store.

Note that times greater than 24 hours are shown by the number of days.

Figure 9. The Timer window.

SAFEPAQ-II can be closed down by clicking the File|Exit… menu item.

Much of the information shown in the Settings window (Figure 1) is stored in the Windows registry so that it is available when SAFEPAQ-II is restarted. In addition the location of the more commonly used windows on the desktop is stored when the window is closed, and then used to position the window when it is reopened.

The windows that have this feature are: SAFEPAQ-II (Figure 2), Log (Figure 6), Targets and sources (Figure 63), Data visualisation (Figure 64), Reaction data (Figure 66), Cache contents (Figure 75), Data selection (Figure 78), Integral C/E (Figure 89), Integral C/E graph (Figure 92), Quality scores (Figure 118), Single reaction processing (Figure 119), Validation plots (Figure 127), Validation plot (Figure 128),Validation data (Figure 129),Validation plot (A) (Figure 130),Validation plot (Q) (Figure 131) and REPORT (Figure 134).

In many of the SAFEPAQ-II windows the text and list boxes are enabled for automatic ‘drag-and-drop’. If the text is selected then it is possible to ‘drag’ this to another application such as a text editor or spreadsheet for further use. This feature is not mentioned for each window, so the user should experiment to see if it is present. As an example, in Figure 10 if a nuclide is selected then dragged out of SAFEPAQ-II, the icon changes to a ‘Cannot drop’, and then when over, say a text editor, it changes to a ‘Pointer with copy’ icon. Releasing the mouse button will place the nuclide name and source in the application.

SAFEPAQ-II has been used to generate all the EAF-2007 libraries; details of these are available in references 9 – 13. As can be seen in Figure 8, the current version of SAFEPAQ-II is 1.0, build 288.

Decay data

The first task when building a new EAF project is to deal with the choice of required nuclides and their decay data.

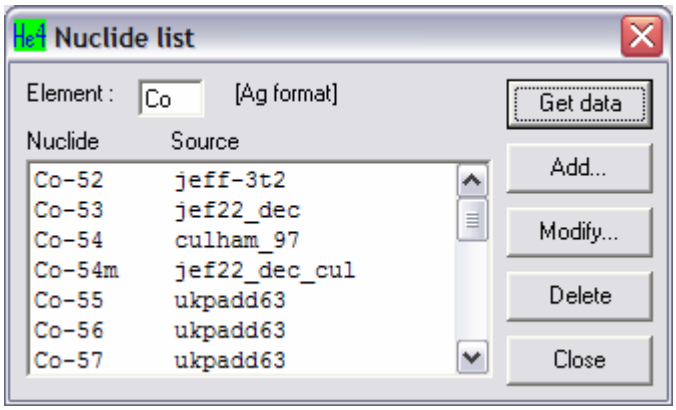


Figure 10. The Nuclide list window.

The sources of data for the nuclides of each element can be viewed in the Nuclide list window shown in Figure 10. This is displayed by clicking on the Decay data|Nuclide list… menu item or the third toolbar button from the right. Enter the symbol for the element and click the Get data button. The data source for a selected nuclide can be modified by clicking the Modify… button to display the Modify nuclide window shown in Figure 11. Note that you need to decide if the nuclide will be considered as a target in the cross section library by ticking the Target check box. Click the Modify button in Figure 11 to save the change.

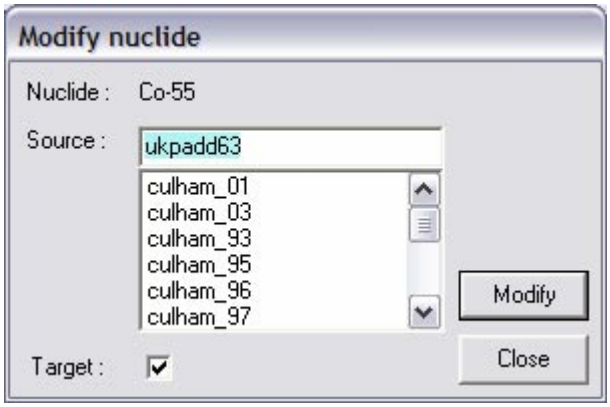


Figure 11. The Modify nuclide window.

A selected nuclide can be removed from the nuclide list by clicking the Delete button in Figure 10, and a new nuclide can be added by clicking the Add… button. This displays the Add nuclide window shown in Figure 12. A new nuclide, its source and whether it is a cross section target are entered and the Add button is clicked to store the changes.

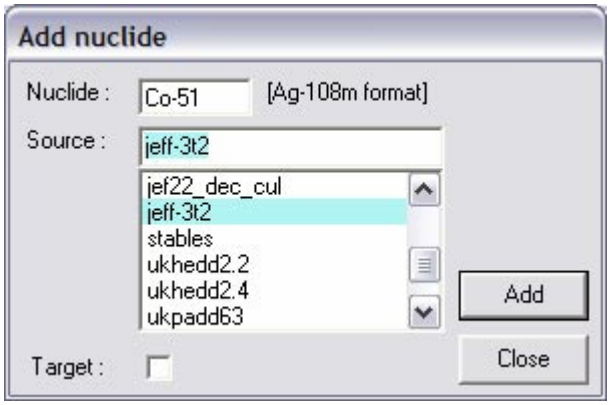


Figure 12. The Add nuclide window.

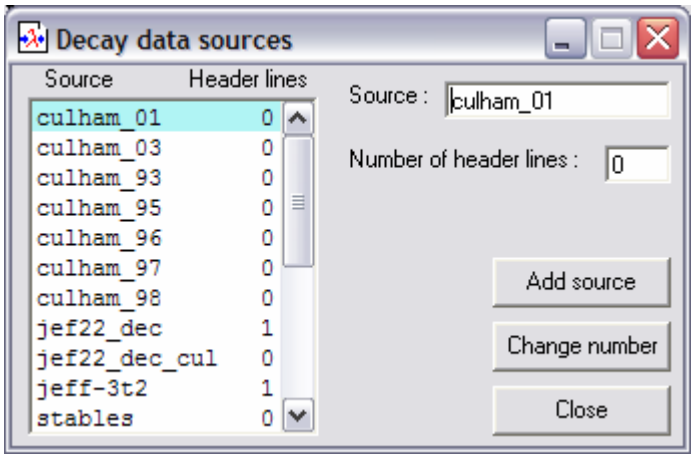


Figure 13. The Decay data sources window.

Changes to the sources can be made using the Decay data sources window shown in Figure 13. This is displayed by clicking on the Decay data|Sources… menu item. A new source can be added by entering the name and clicking the Add source button. The number of header lines for an existing source can be changed by entering the number and clicking the Change number button. All the decay data sources are held in the folder specified in the Decay data folder text box in the Settings window (Figure 1) in standard ENDF format. In contrast to the cross section libraries these are not converted to databases. The reason is that no modifications are made to the decay data; only a choice from various sources is made. If a new source of data is available, and it is required that all nuclides originally with source *old_source* are changed to *new_source*, then the Global source replace window shown in Figure 14 can be used. This is displayed by clicking on the Decay data|Global source replace… menu item. The old and new source names are entered in the text boxes and by clicking the Replace button the changes are made.

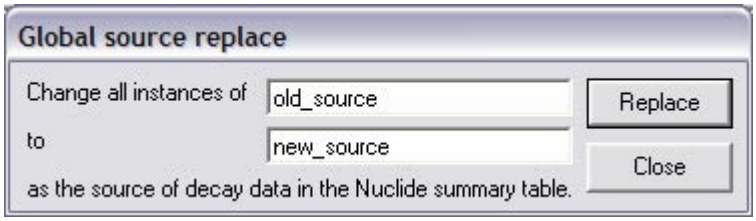


Figure 14. The Global source replace window.

The biological hazard data in the *KnownHazards* table can be viewed and altered by clicking the Decay data|Known hazard data… menu item. This displays the Known hazard data window shown in Figure 15. Selecting a nuclide from the dropdown list displays ingestion and inhalation coefficients and the source of data. Data for a new nuclide can be entered by clicking the Add button, which causes all four text boxes to be blank (with a white background) ready for data entry. Click the Save button to save the new data or the Cancel button (in the same place as the Close button) to remove the new data. Data values can be changed by selecting the nuclide and clicking the Modify button, this makes the background of the final three text boxes white and enables the Save button. Data for a nuclide can be removed by clicking the Delete button. Prior to any data changes being made a confirmation dialog is displayed.

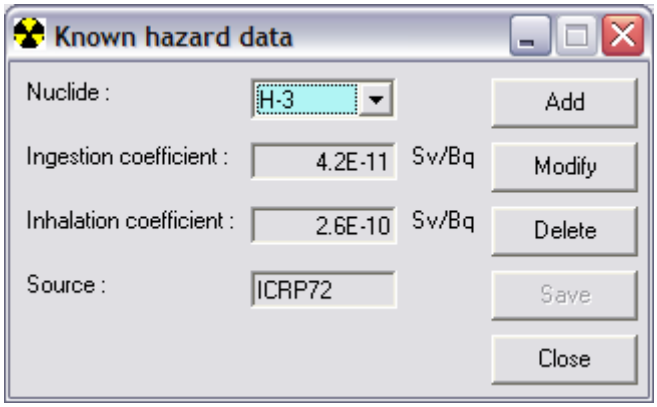


Figure 15. The Known hazard data window.

The A_2 data in the *A2_IAEA* table can be viewed and altered by clicking the Decay data|Known A2 data… menu item. This displays the Known A2 data window shown in Figure 16. Selecting a nuclide from the dropdown list displays its A_2 value and the source of data. Data for a new nuclide can be entered by clicking the Add button, which causes all three text boxes to be blank (with a white background) ready for data entry. Click the Save button to save the new data or the Cancel button (in the same place as the Close button) to remove the new data. Data values can be changed by selecting the nuclide and clicking the Modify button, this makes the background of the final two text boxes white and enables the Save button. Data for a nuclide

can be removed by clicking the Delete button. Prior to any data changes being made a confirmation dialog is displayed.

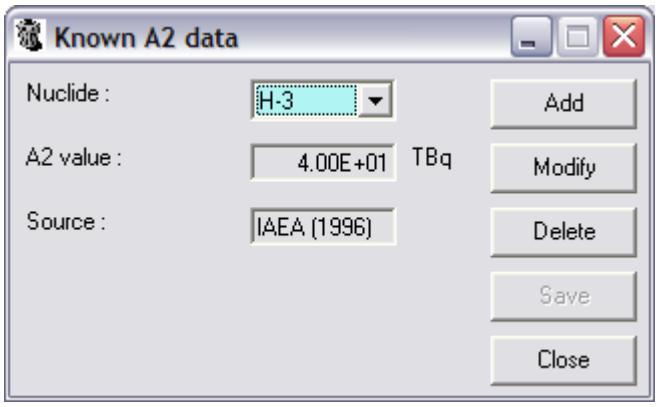


Figure 16. The Known A2 data window.

The clearance data in the *Clearance_IAEA* table can be viewed and altered by clicking the Decay data|Known clearance data… menu item. This displays the Known clearance data window shown in Figure 17. Selecting a nuclide from the dropdown list displays its clearance level value. The default unit for the clearance level is $Bqkg^{-1}$. However, by clicking the # button data are displayed (and entered) as Bqg^{-1}. Note that this button acts as a toggle and pressing it again will revert to the default unit. Data for a new nuclide can be entered by clicking the Add button, which causes the two text boxes to be blank (with a white background) ready for data entry. Click the Save button to save the new data or the Cancel button (in the same place as the Close button) to remove the new data. Data values can be changed by selecting the nuclide and clicking the Modify button, this makes the background of the final text box white and enables the Save button. Data for a nuclide can be removed by clicking the Delete button. Prior to any data changes being made a confirmation dialog is displayed.

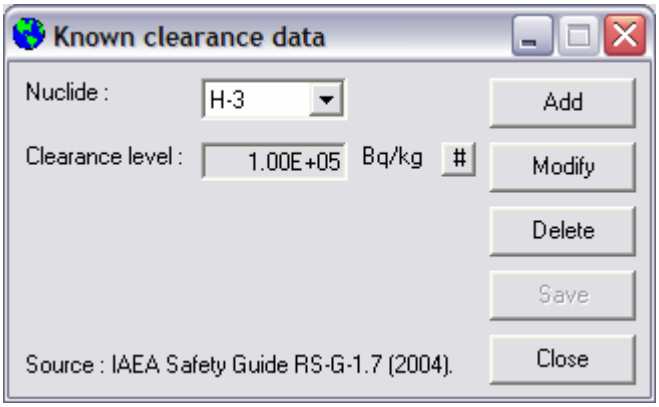


Figure 17. The Known clearance data window.

Information on the spins of the ground state and isomers should be available when producing the cross section library. In some poorly known nuclides the spin is unknown, such a lack of data could cause problems. These nuclides can be identified by clicking on the Decay data|Find nuclides with unknown spin… menu item. This displays the Nuclides (isomers) with unknown spin window shown in Figure 18. It is recommended that these nuclides be investigated and the spin data improved.

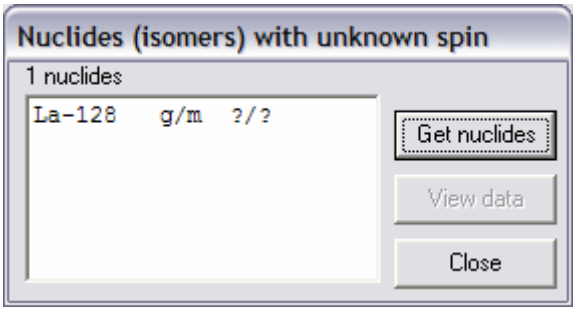


Figure 18. The Nuclides (isomers) with unknown spin window.

Once all nuclides and the data sources are specified then the data can be assembled by clicking on the Decay data|Assemble decay data… menu item. This displays the Assemble decay data window shown in Figure 19. The file name that was entered in the New EAF project window (Figure 3) is automatically entered in the File name text box (it is recommended that this should not be changed). This name is used to construct the names of the various decay data files. Tick the various check boxes in the Processes group and click the Assemble button to begin the assembly process. This is quick (~ 1 minute) and all the decay data files required by FISPACT are generated. The second option generates the *DecayData* table in Parameter that contains all the decay data; this is required for subsequent cross section processing.

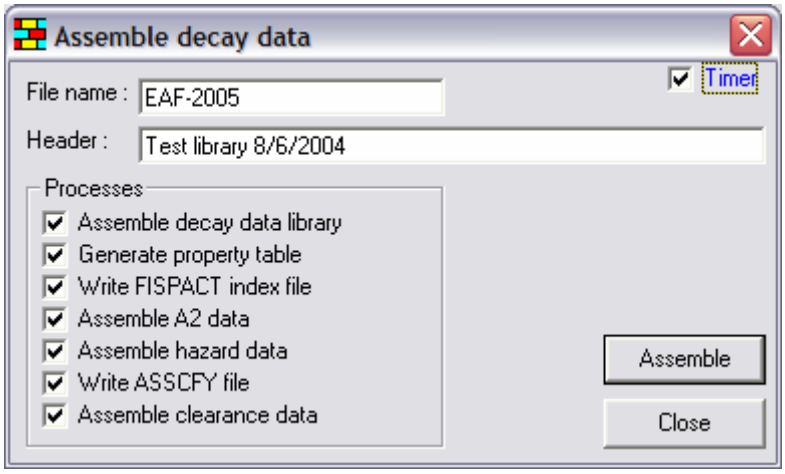


Figure 19. The Assemble decay data window.

Clicking the Decay data|Documentation menu item will write two files `decay_library_contents` and `hazard_library_contents` (in the folder specified in the Decay data folder textbox in the Settings window (Figure 1). These contain the decay data in a readable format suitable for use in the EAF reports.

The decay data held in the *DecayData* table of the Parameter database can be inspected by clicking the Decay data|Decay data viewer… menu item or the second toolbar button from the right. This opens the Decay data viewer window shown in Figure 20. This has a menu bar and a toolbar, and when a nuclide is entered in the text box and the Get data button clicked (or the first toolbar button clicked or the Enter key pressed) data for the nuclide are displayed. The nuclide symbol is displayed at the top centre, the colour of the background indicates the decay mode (a key to these colours is shown in Figure 20, having been made visible by clicking the Key >> button, it can be removed by clicking the Key << button). Selecting from the dropdown list boxes alters the units for half-life and energy. Clicking the Photon lines or Matter lines tabs displays further information on the emitted photons and particles.

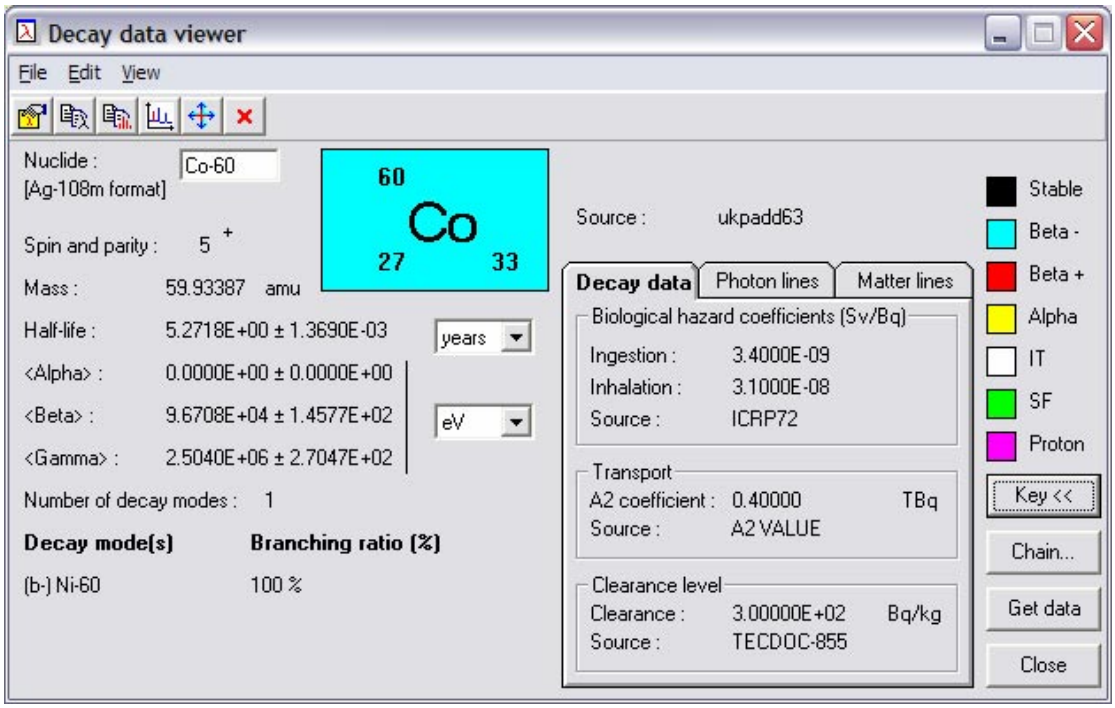


Figure 20. The Decay data viewer window.

Clicking the Edit|Copy decay data menu item or the second toolbar button places the information displayed on the main widow and the Decay tab on the clipboard, clicking the Edit|Copy line data menu item or the third toolbar button places the information displayed on the Photon lines and

Matter lines tabs on the clipboard. Clicking the fifth toolbar button (Navigator) changes the nuclide symbol box so that nine nuclides are shown – the current nuclide and the eight that surround it in a 'Chart of the Nuclides' plot. Clicking one of these makes that nuclide the current one, displaying data for it.

Clicking the Chain… button displays the Decay chain window shown in Figure 21 (the nuclide name is placed in the title bar of the window). Clicking the Draw menu item displays the chains, by default with no half-life information in black and white. Clicking the Options|Colour menu item shows the arrows in the colours appropriate for the decay mode (the key colours in Figure 20), while clicking the Options|Show half-life menu item includes the nuclide half-lives (as shown in Figure 21). The Options|Font and Options|Size menu items allow the size (6, 8, 10 points) and font type (Courier or Times) to be used to display the chains. Clicking the Print menu item sends the displayed decay chain to the default printer, while the Close menu item closes the window. If the length of the chains is such that not all are visible in the window then the window can be resized or the > and << menu items can be used to scroll the contents of the window.

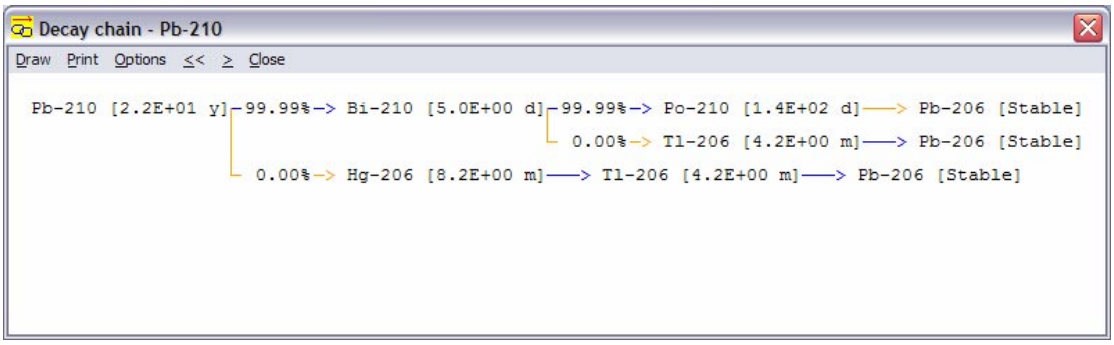


Figure 21. The Decay chain window.

Clicking the View|Plot line energies… menu item in Figure 20 or the fourth toolbar button displays the Line spectrum window shown in Figure 22. This plots the gamma and X-ray lines (in blue and red respectively) that are emitted by the nuclide. The graph can be printed to the default printer by clicking the File|Print menu item and it can be copied to the clipboard by clicking the Edit|Copy menu item. The graph is 'Hot', by clicking on the top of any of the lines information about it is displayed in the status bar.

In SAFEPAQ the nuclides and their sources were available in a set of files. In SAFEPAQ-II this information is stored in tables in the Parameter database. To enable the existing files to be read a series of reading routines are available. These are accessed from the Decay data menu. The location of the files is the folder `ascii` on the disk shown in the Source database disk text box in the Settings window (Figure 1).

- Clicking on the Decay data|Read nuclides file menu item reads the `nuclides.asc` file and enters the data into the database.
- Clicking on the Decay data|Read additional stables data menu item reads the `stables_additional` file and enters the data into the database.
- Clicking on the Decay data|Read A2 file menu item reads the `a2_iaea.asc` file and enters the data into the database.
- Clicking on the Decay data|Read Hazard file menu item reads the `known_haz.asc` file and enters the data into the database.
- Clicking on the Decay data|Read Wapstra mass table menu item reads the `wapstra-masstable` file and enters the data into the database.

These data are already present in the Parameter database, so the above methods should not be used for routine modification of the nuclides. A series of windows are available to display and edit the reactions and data (Figure 10 - Figure 17). This is the recommended method of making changes to the data for the nuclides, as all changes will be logged.

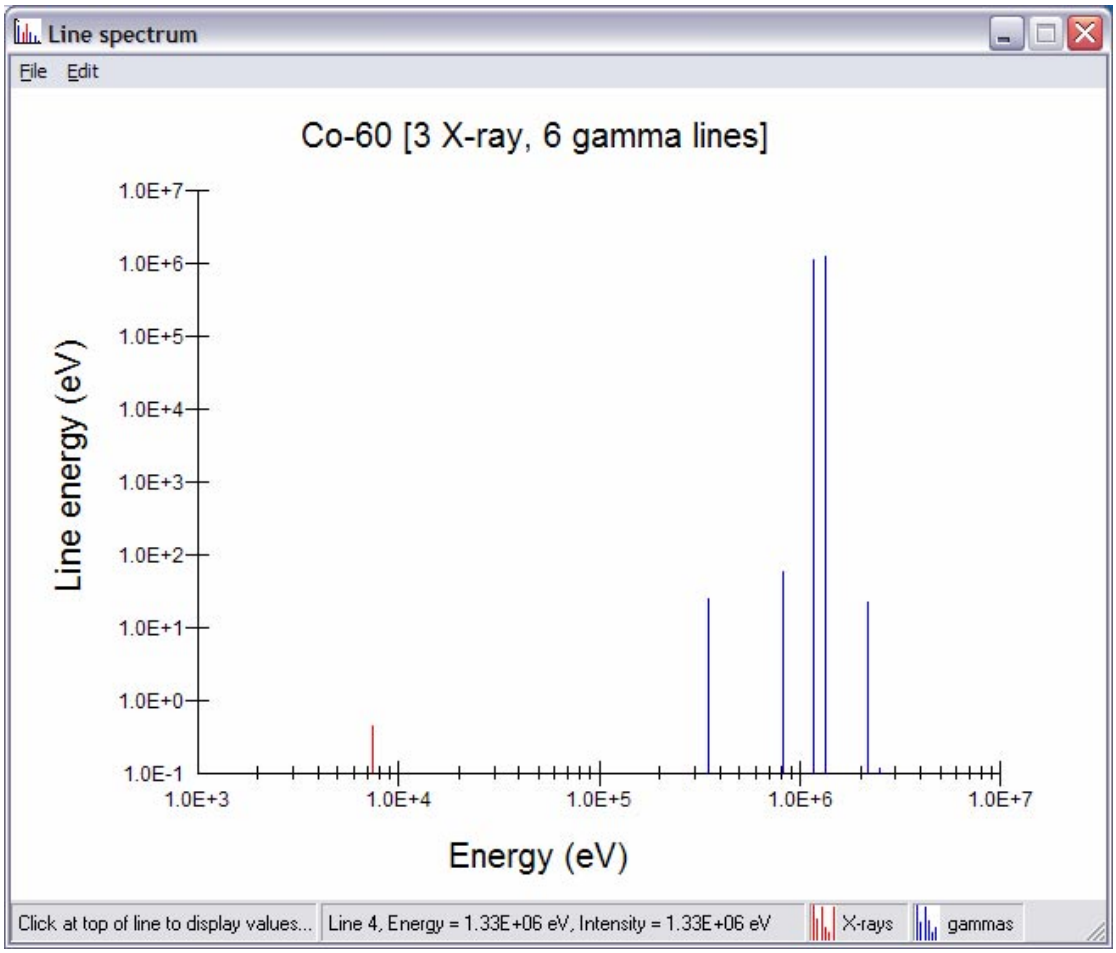


Figure 22. The Line spectrum window.

Source libraries

The first step in the construction of an EAF cross section library is to read all the various source libraries. These source libraries are read and converted to a standard database structure. Details of the libraries are stored in the Library database. Because the source files may be in various formats the reading options must be specified. Click on Libraries|Library options… or the twenty-first toolbar button to display the Library options window shown in Figure 23.

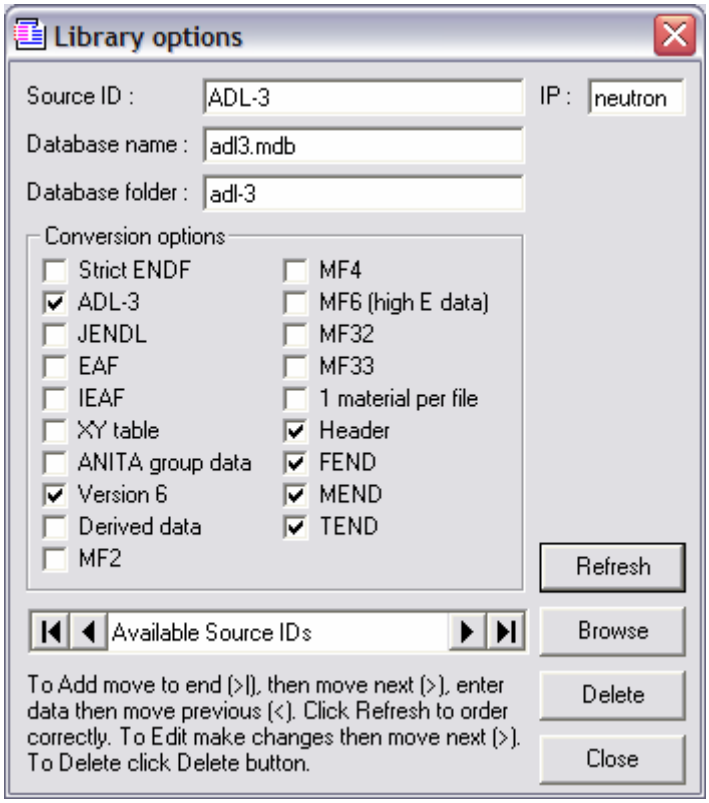


Figure 23. The Library options window.

The options for the existing sources are shown by a series of check boxes in the Conversion options group. Text in the window gives instructions on how to add or edit source details, source details can be removed by clicking the Delete button. Note that deleting does not remove the basic data which are held in a database for the library; but only the details about the source, which are held in the Library database. The Browse button displays the Open dialog that allows the database location to be specified. Some degree of experimentation will be necessary to select the various Conversion options. These specify the type of file (ENDF, version, EAF, ADL, JENDL, IEAF, XY table, ANITA group data or with derived data), what types of data are present (MF = 2, 4, 6, 32, 33), if there is a header line, if the various ENDF end lines are present (FEND, MEND and TEND) and whether the file (or files) contains

more that one material per file. Note that from EAF-2007, projects with an incoming particle other than a neutron can be used. The incoming particle (IP) text box allows the type of library (neutron, proton or deuteron) to be specified.

If a new library has been specified in the Library options window, then data can be read by clicking on Libraries|Read new library… or the eighteenth toolbar button to display the Read new library window shown in Figure 24. Select the required Source ID and click Read to read and convert the data. Note that if the database already exists then you are given the option to delete it, copy the generic database, rename it and then read in the data. Note that the data file(s) are assumed to be in the same folder as the corresponding database.

A summary of all the available source libraries can be seen by displaying the Library summary window shown in Figure 25. This is displayed by clicking on the Libraries|Library summary… menu item or the twentieth toolbar button. This shows the available sources, the conversion options used and the types and numbers of reactions. Having read a new library using Figure 24 it is necessary to add this to the summary by clicking the Add… button in Figure 25. This displays the Add library window shown in Figure 26. Any libraries not entered into the summary are displayed; clicking the Add button will add the selected library.

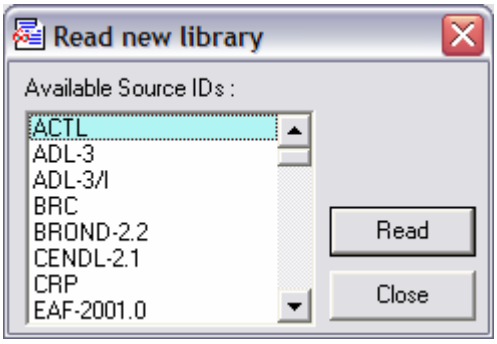


Figure 24. The Read new library window.

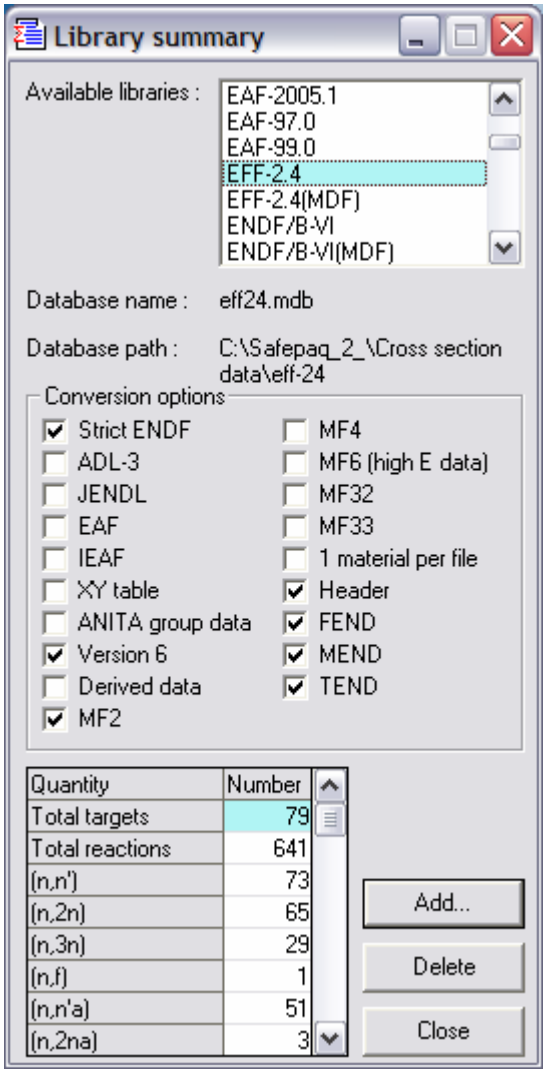


Figure 25. The Library summary window.

Note that if you wish to re-read a source library then it is necessary to first remove it from the summary using the Delete button in Figure 25, then to read it using Figure 24 and then to add it to the summary again using Figure 25 and Figure 26.

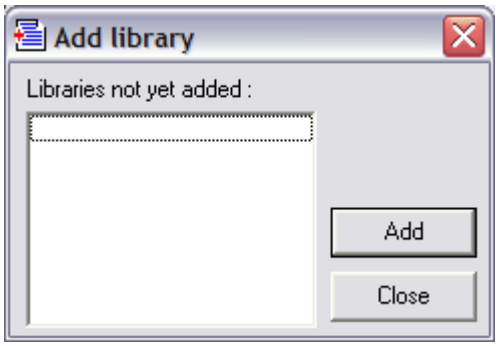


Figure 26. The Add library window.

The Library summary window can be used to check what data are contained in each library, but if it is required to check which

libraries contain a particular reaction, then it is quicker to use the Library search window shown in Figure 27. This is displayed by clicking on the Libraries|Library search… menu item or the nineteenth toolbar button. It is possible to enter various amounts of information before making the search by clicking the Find button. Note that only libraries appropriate to the type of incoming particle selected in the Settings window (Figure 1) are displayed. If the Target element is specified (the three remaining boxes are empty) then libraries containing that element as a target are displayed. If the Target element and Target mass are specified (the two remaining boxes are empty) then libraries containing that nuclide in any isomeric state as a target are displayed. If the Target element, Target mass and Target state are specified (the Reaction box is empty) then libraries containing that nuclide as a target are displayed. If all the inputs are specified then libraries containing that nuclide as a target for that reaction are displayed. Note that you cannot 'leave gaps' in the input, if a reaction is specified then all the three boxes above must be filled. The result of the search process can be copied to the clipboard by clicking the Copy button.

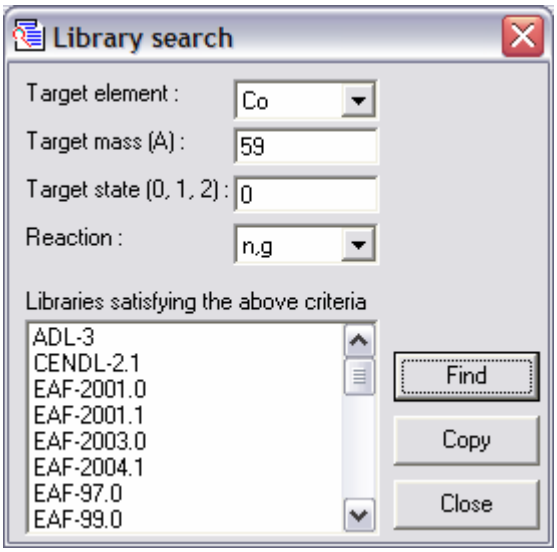


Figure 27. The Library search window.

In most cases it is possible to use data from the original source libraries in constructing the new EAF library. However, for some reactions it is preferrable to use data that have been specially prepared for a previous EAF library. In such a case data can be extracted from an existing Master Data File (MDF) that was prepared using SYMPAL. The whole MDF should be stored in the folder `MDF` on the Source database disk, and Cross section data folder specified in the Settings window (Figure 1). The Extract data from MDF window shown in Figure 28 is used to extract the data. This is displayed by

clicking on the Libraries|Extract data from MDF… menu item. The name of the MDF is entered in the first text box, the name of the file where the extracted data are to be put is given in the second text box and the name of the Source ID (the name used in Figure 23) is entered in the third. Clicking the Extract button will read the whole MDF and copy data for the Source ID into the new file. This can then be used as an additional source in the same way as any of the existing source libraries.

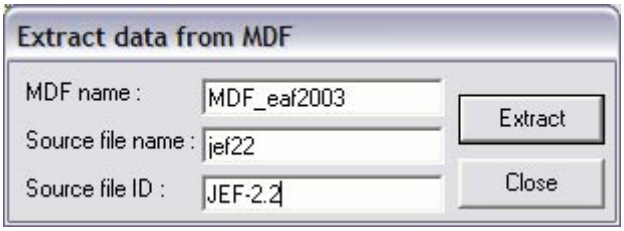


Figure 28. The Extract data from MDF window.

Experimental data

In SYMPAL the collection of selected experimental data was held in a set of specially formatted 'ASCII' tables. In SAFEPAQ-II these data are stored in tables in the Parameter database. To enable the existing ASCII tables to be read a series of reading routines are available. These are accessed from the Experimental data menu. The location of the ASCII files is the folder `ascii` on the Source database disk specified in the Settings window (Figure 1).

- Clicking on the Experimental data|Read experimental data menu item reads the `expi.asc` file and enters the data into the database.
- Clicking on the Experimental data|Read systematics data menu item reads the `systrn.asc` file and enters the data into the database.
- Clicking on the Experimental data|Read uncertainty data menu item reads the `ngeh-ev-unc.asc`, `nfeh-ev-unc.asc` and `nXX-unc.asc` files and enters the data into the database.
- Clicking on the Experimental data|Read resonance integral data menu item reads the `resina.asc`, `resinf.asc`, `resing.asc` and `resinp.asc` files and enters the data into the database.

These data are already present in the Parameter database, so the above methods should not be used for routine modification of the experimental data. A series of windows (Figure 29 - Figure 42) are available to display and edit the experimental data. This

is the recommended method of making changes to the experimental data, as all changes will be logged.

The data available at thermal energy can be displayed by clicking on Experimental data|View 0.0253 eV data … or the tenth toolbar button to display the 0.0253 eV experimental data window shown in Figure 29. Selecting a target shows which reactions have data, and selecting a reaction displays the available data in the grid. Note that depending on the incoming particle type selected the Settings window (Figure 1) the reactions here and in subsequent windows will be e.g. (n,2n), (d,2n) or (p,2n). In addition to the energy, cross section and uncertainty displayed in the first three columns, the last three columns show three flags. These indicate whether the data are used for calculating branching modifications (Use B), for calculating renormalisation modifications (Use R) and in validation (Use V). The source of the data is indicated by a reference, where this is known. Clicking the Modify button will display the selected data in editing boxes below the reference. Changes to the data values or the flags can then be made and saved to the database by clicking the Save button. A new data point can be added by clicking the Add button. This displays the dialog shown in Figure 30, asking if the new data point is for the selected target and reaction. If the Yes button is clicked then the editing boxes used in the modification process are used. If the No button is clicked then the Add 0.0253 eV experimental data window shown in Figure 31 is displayed.

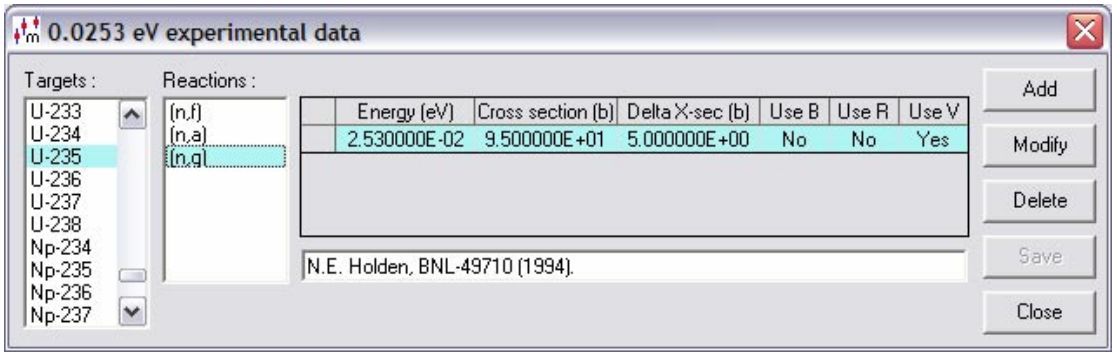


Figure 29. The 0.0253 eV experimental data window.

Enter target and reaction details in the first text box, the dropdown list and with the Final state radio buttons. Enter the experimental data in the text boxes and check the usage flags that apply. The default cross section unit is b, but by clicking the # button it is possible to toggle between b and mb for data entry. Note that the # button should be clicked prior to data entry. Select a reference from the dropdown list. Clicking the Add button will save the data in the Parameter database. Note that the flags must be chosen so that either none or only a single data point is used for branching, renormalisation or validation.

However, if duplicates are present then the last entered 'Yes' value is retained, any existing 'Yes' is automatically changed to 'No'.

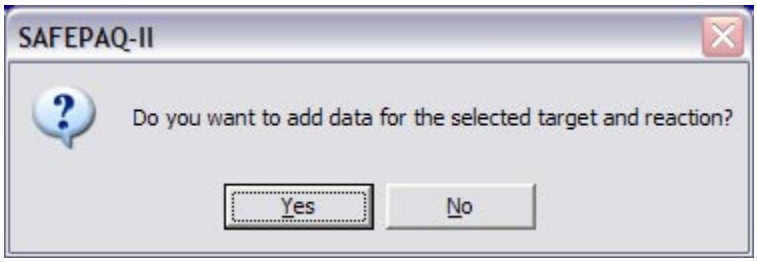


Figure 30. A dialog to choose the type of Add process.

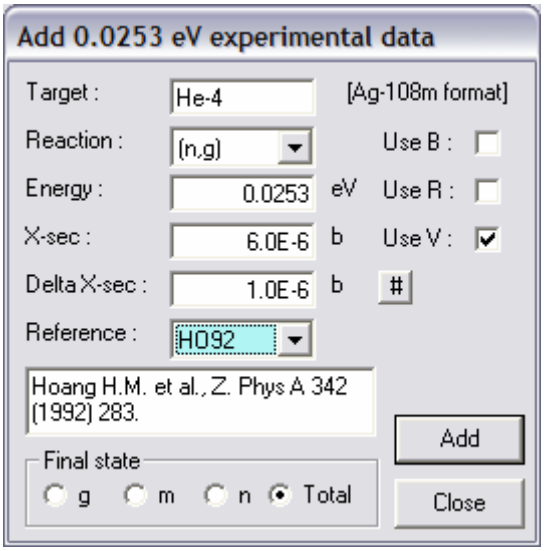


Figure 31. The Add 0.0253 eV experimental data window.

The data available at 30 keV can be displayed by clicking on Experimental data|View 30 keV data … or the eleventh toolbar button to display the 30 keV experimental data window shown in Figure 32. Selecting a target shows which reactions have data, and selecting a reaction displays the available data in the grid. In addition to the energy, cross section and uncertainty displayed in the first three columns, the last three columns show three flags. These indicate whether the data are used for calculating branching modifications (Use B), for calculating renormalisation modifications (Use R) and in validation (Use V). The source of the data is indicated by a reference, where this is known. Clicking the Modify button will display the selected data in editing boxes below the reference (shown in Figure 32). Changes to the data values or the flags can then be made and saved to the database by clicking the Save button; if the change is not required then click the Cancel button. A new data point can be added by clicking the Add button. This displays the dialog shown in Figure 30, asking if the new data point is for the selected target and

reaction. If the Yes button is clicked then the editing boxes used in the modification process are used. If the No button is clicked then the Add 30 keV experimental data window, very similar to that shown in Figure 31, is displayed. Note that the flags must be chosen so that either none or only a single data point is used for branching, renormalisation or validation. However, if duplicates are present then the last entered 'Yes' value is retained, any existing 'Yes' is automatically changed to 'No'.

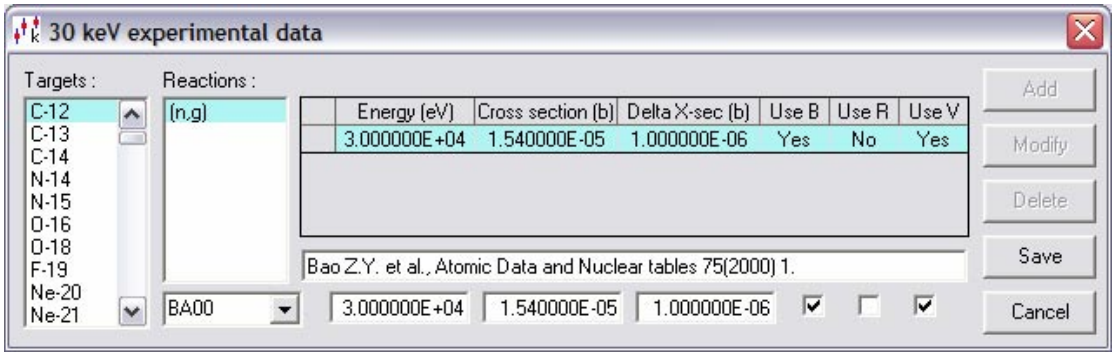


Figure 32. The 30 keV experimental data window.

The data available at 14.5 MeV can be displayed by clicking on Experimental data|View 14.5 MeV data … or the twelfth toolbar button to display the 14.5 MeV experimental data window shown in Figure 33. Selecting a target shows which reactions have data, and selecting a reaction displays the available data in the grid. In addition to the energy, cross section and uncertainty displayed in the first three columns, the last three columns show three flags. These indicate whether the data are used for calculating branching modifications (Use B), for calculating renormalisation modifications (Use R) and in validation (Use V). The source of the data is indicated by a reference, where this is known. Clicking the Modify button will display the selected data in editing boxes below the reference. Changes to the data values or the flags can then be made and saved to the database by clicking the Save button. A new data point can be added by clicking the Add button. This displays the dialog shown in Figure 30, asking if the new data point is for the selected target and reaction. If the Yes button is clicked then the editing boxes used in the modification process are used. If the No button is clicked then the Add 14.5 MeV experimental data window, very similar to that shown in Figure 31, is displayed. Note that the flags must be chosen so that either none or only a single data point is used for branching, renormalisation or validation. However, if duplicates are present then the last entered 'Yes' value is retained, any existing 'Yes' is automatically changed to 'No'.

At this energy there are typically many reactions on a target, and several data points for a given reaction.

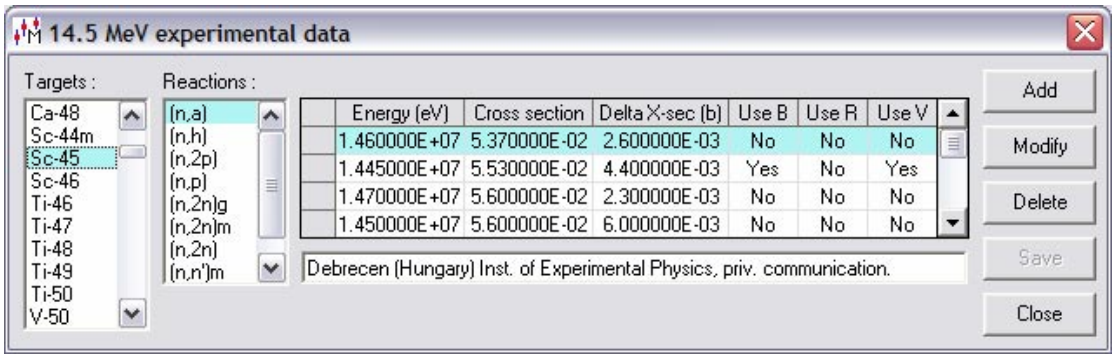


Figure 33. The 14.5 MeV experimental data window.

The data available for the resonance integal can be displayed by clicking on Experimental data|View RI data … or the thirteenth toolbar button to display the RI experimental data window shown in Figure 34. Selecting a target shows which reactions have data, and selecting a reaction displays the available data in the grid. In addition to the resonance integral and uncertainty displayed in the first two columns, the last three columns show three flags. These indicate whether the data are used for calculating branching modifications (Use B), for calculating renormalisation modifications (Use R) and in validation (Use V). Clicking the Modify button will display the selected data in editing boxes below the reference. Changes to the data values or the flags can then be made and saved to the database by clicking the Save button. A new data point can be added by clicking the Add button. This displays the dialog shown in Figure 30, asking if the new data point is for the selected target and reaction. If the Yes button is clicked then the editing boxes used in the modification process are used. If the No button is clicked then the Add RI experimental data window, very similar to that shown in Figure 31, is displayed. Note that the flags must be chosen so that either none or only a single data point is used for branching, renormalisation or validation. However, if duplicates are present then the last entered 'Yes' value is retained, any existing 'Yes' is automatically changed to 'No'. Note that at present no resonance integral data are used for renormalisation or branching.

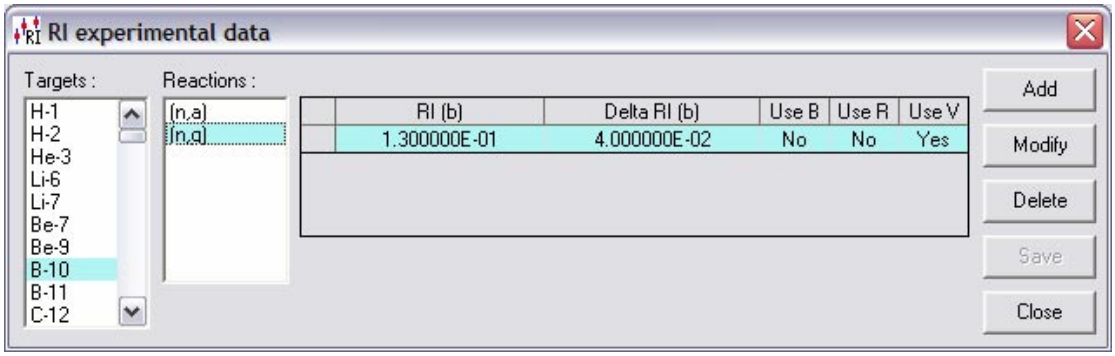


Figure 34. The RI experimental data window.

The uncertainty data for non-threshold reactions can be displayed by clicking on Experimental data|View non-threshold uncertainty data… or the fourteenth toolbar button to display the Non-threshold uncertainty data window shown in Figure 35. Click on a target to show the reactions present. Click on a reaction to display the uncertainty data. These data cannot be changed until the Modify button is clicked. Then click on the Save button to save the change to the Parameter database. If the change is not required then click the Cancel button. Data for a reaction can be removed from the database by clicking the Delete button. To add new uncertainty data click the Add… button, which displays the Add non-threshold uncertainty window shown in Figure 36.

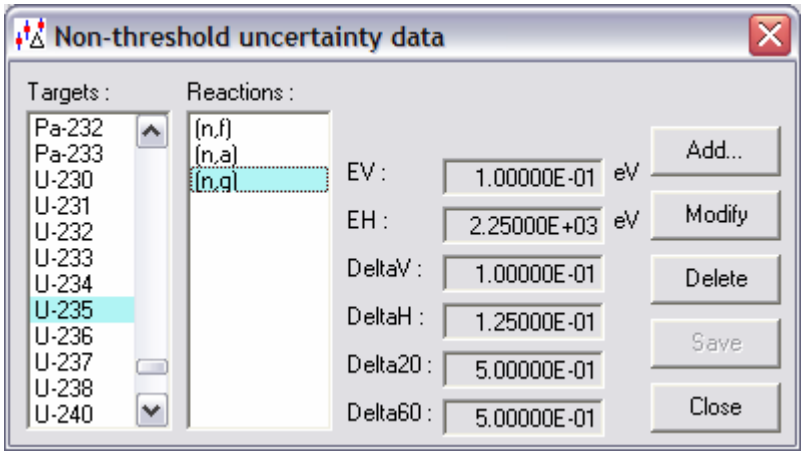


Figure 35. The Non-threshold uncertainty data window.

In Figure 35 the four (three for a non-extended library) 'Delta' values are shown. Delta (Δ) is defined as $\Delta\sigma/\sigma$, where $\Delta\sigma$ is the uncertainty in cross section and the error factor (f) is defined as $f = 1 + \Delta$.

In Figure 36 enter the target in the first text box, select the reaction from the dropdown list and enter the six (five for a non-extended library) required values in the remaining text

boxes. Select a final state from the radio buttons and click the Add button to save the values in the database.

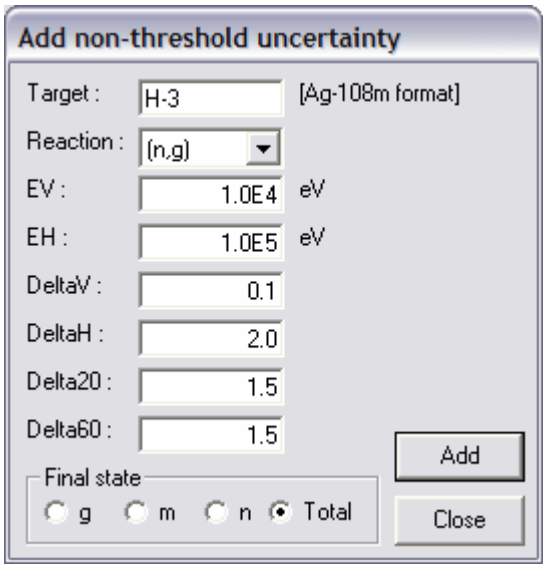


Figure 36. The Add non-threshold uncertainty window.

It is necessary that all (n,γ) and (n,f) reactions have uncertainty data (specifically E_V and E_H values). Prior to starting to build the EAF library this can be checked by clicking on the Experimental data|Find reactions with no non-threshold uncertainty data… menu item to display the Reactions with no uncertainty data window shown in Figure 37. Any displayed reactions should have uncertainty data added.

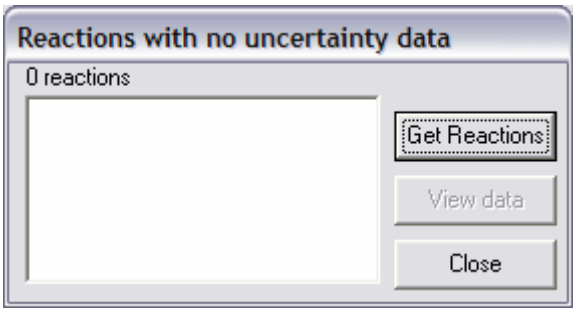


Figure 37. The Reactions with no uncertainty data window.

The uncertainty data for threshold reactions can be displayed by clicking on Experimental data|View threshold uncertainty data… or the fifteenth toolbar button to display the Threshold uncertainty data window shown in Figure 38. Click on a target to show the reactions present. Click on a reaction to display the uncertainty values. These values cannot be changed until the Modify button is clicked. Then click on the Save button to save the change to the Parameter database. If the change is not required then click the Cancel button. Data for a reaction can be removed from the database by clicking the Delete button. To add a new uncertainty value click the Add…

button, which displays the Add threshold uncertainty window shown in Figure 39.

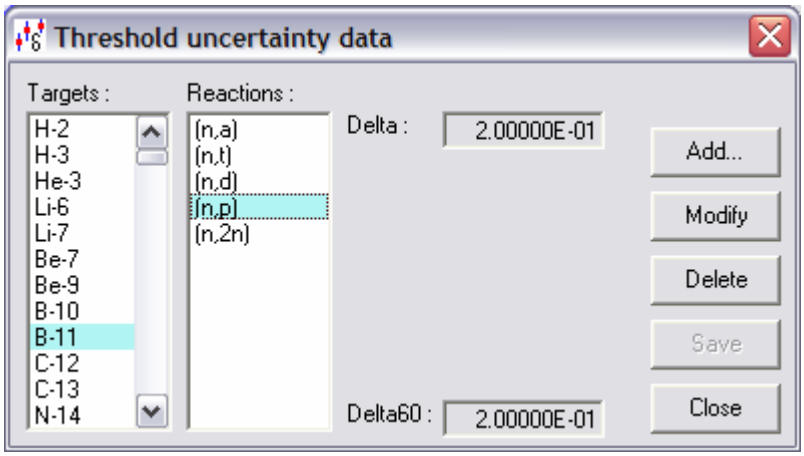


Figure 38. The Threshold uncertainty data window.

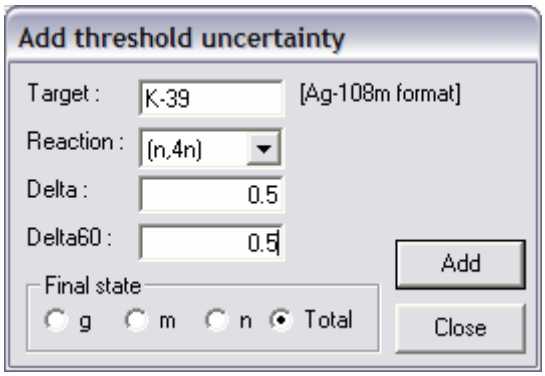


Figure 39. The Add threshold uncertainty window.

Enter the target in the first text box, select the reaction from the dropdown list and enter the required values in the remaining two (one for a non-extended library) text boxes. Select a final state from the radio buttons and click the Add button to save the value in the database.

The experimental data contain references to the source of the data. These references are held in the Parameter database and can be viewed by clicking on Experimental data|View References … or the seventeenth toolbar button to display the References window shown in Figure 40. A Source ID and the reference text are shown. As indicated by the window text it is possible to add a new reference or edit an existing one. Editing is done by changing the text. Note that the Source ID should **not** be changed.

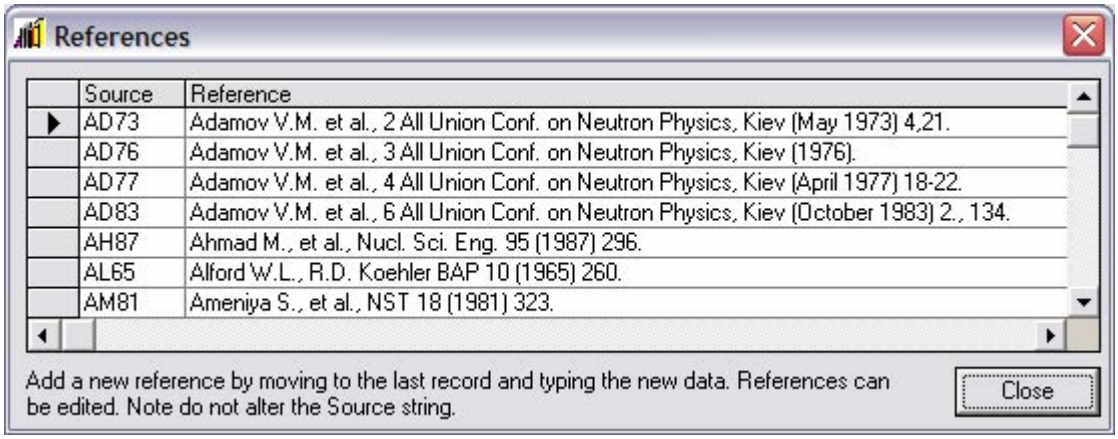

References
Source
Reference
AD73
Adamov V.M. et al., 2 All Union Conf. on Neutron Physics, Kiev (May 1973) 4,21.
AD76
Adamov V.M. et al., 3 All Union Conf. on Neutron Physics, Kiev (1976).
AD77
Adamov V.M. et al., 4 All Union Conf. on Neutron Physics, Kiev (April 1977) 18-22.
AD83
Adamov V.M. et al., 6 All Union Conf. on Neutron Physics, Kiev (October 1983) 2., 134.
AH87
Ahmad M., et al., Nucl. Sci. Eng. 95 (1987) 296.
AL65
Alford W.L., R.D. Koehler BAP 10 (1965) 260.
AM81
Ameniya S., et al., NST 18 (1981) 323.
Add a new reference by moving to the last record and typing the new data. References can be edited. Note do not alter the Source string.
Close

Figure 40. The References window.

Under the Experimental data menu there is an item to view those nuclides for which systematics data are used during renormalisation. If the flags are set then systematics take precedence over any experimental data. The systematics flags can be seen by clicking the Experimental data|View systematics flags … menu item, this opens the Systematics flags window shown in Figure 41.

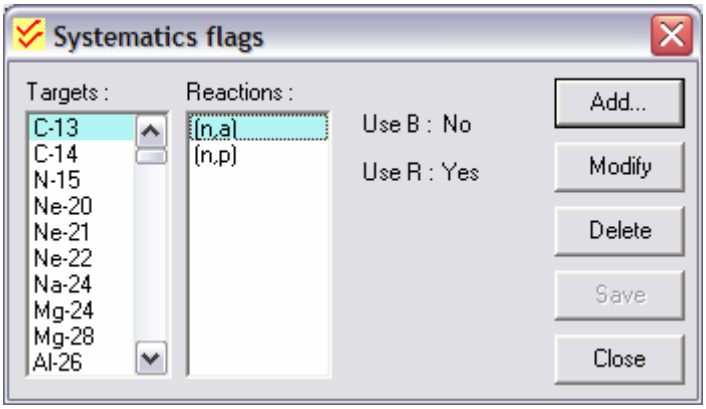


Figure 41. The Systematics flags window.

Clicking the Modify button displays check boxes for the two flags, clicking the Save button will store the new values in the database. Clicking the Delete button removes the selected reaction from the database. Clicking the Add… button displays the Add systematics flags window shown in Figure 42. Use the text box and dropdown list to select the reaction, use the radio buttons to select the final state and set the flags before saving by clicking the Add button. Prior to EAF-2005 systematics flags were only set for Final state = Total. If flags to isomeric states are specified then when used the branching ratio systematic is also applied so that, for example, a renormalistaion can be made to systematics for an isomeric state.

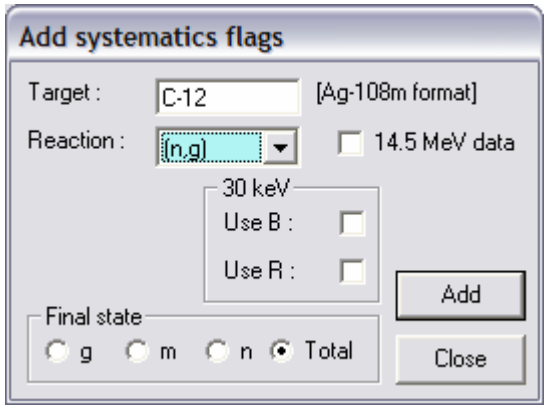


Figure 42. The Add systematics flags window.

In Figure 41, if the selected reaction is (n,γ) then additional data for the 30 keV systematic are displayed. These can be modified in the same way as the 14.5 MeV flags, and in Figure 42, check boxes for these additional flags are displayed if the reaction is (n,γ). Note that as the Use B flag is never used it should always remain unchecked. In Figure 42 this is made explicit as the Use R check box is renamed 14.5 MeV data.

The formulae for the systematics are discussed in the EAF-2007 documentation [10]. For the (n,t), (n,d), (n,n′p) and (n,n′p+d) reactions an alternate set of formulae have been defined. The choice between the two set can be made by selecting Standard or Alternate on the Experimental data|Systematics menu item. Note that this choice remains until changed and so applies to all calculation or use of systematics.

Clicking the Experimental data |Elemental analysis… menu item displays the Elemental analysis window shown in Figure 43. The element and reaction are selected from the dropdown lists and the energy, elemental cross section and uncertainty are entered in the text boxes. The required isotope (generally the most abundant) is selected by clicking one of the radio buttons to the left of the table and the Get data button is clicked. The cross sections for the various isotopes are extracted from the Final database at the specified energy and entered in the third column of the table. When all the cross sections have been found then the sum is formed and the k_i values defined in equation (1) are calculated and displayed in the fourth column. In equation (1) the cross sections (σ_i^c) are the library values, while f_i are the abundances. Finally the isotopic cross section value is displayed in the text box.

$$k_i = \sigma_i^c \Big/ \sum_j f_j \sigma_j^c \qquad (1)$$

By default the natural abundances are displayed in the second column. By clicking on the Enriched radio button it is possible

to edit the abundance values to the required values. As can be seen from Figure 43, the isotopic value is generally similar to the elemental value, but this depends on the actual cross sections and abundances of the isotopes for the selected element.

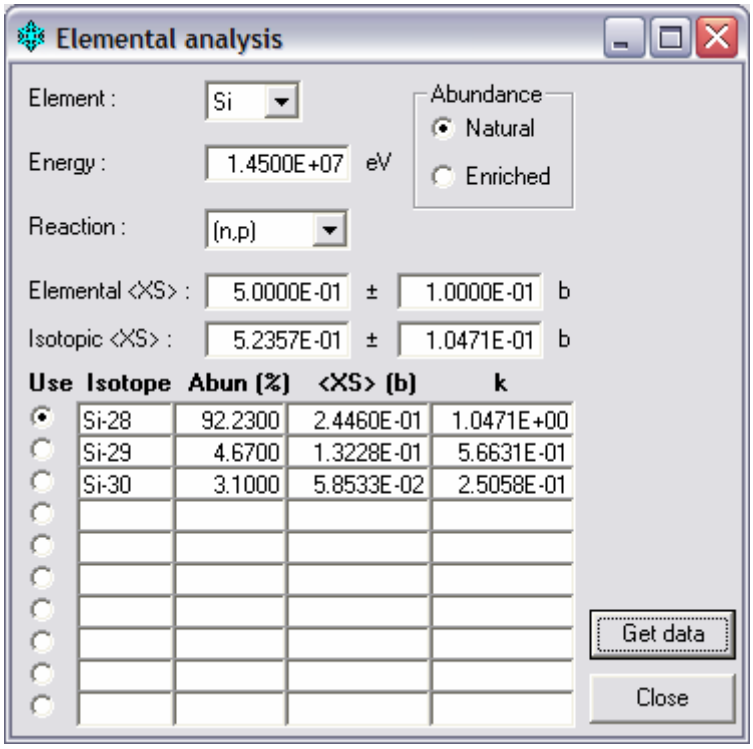


Figure 43. The Elemental analysis window.

EXFOR data

The primary source of experimental data is EXFOR, maintained by the Nuclear Data Centres. The NEA Data Bank have put this on two CD-ROMs and distributed them as part of the JEF-PC package. These CD-ROMs are used by SAFEPAQ-II as the source of EXFOR data. The EXFOR files have been searched in the past and relevant data extracted. As part of the original SAFEPAQ program, provision was made to store the selected data in a set of `*.x4s` files (see Appendix 2). These can be read by SAFEPAQ-II and stored in the EXFOR database. This is done from the EXFOR menu. The location of the `x4s` files is the folder `exfor` on the Source database disk specified in the Settings window (Figure 1).

- Clicking on the EXFOR|Read x4s files menu item reads the `*.x4s` files and enters the data into the database.

These data are already present in the EXFOR database, so the above method should not be used for routine modification of the EXFOR data. Two windows (Figure 45 and Figure 47) are available to display and select the EXFOR data. This is the

recommended method of making changes to the EXFOR data, as all changes will be logged.

The SAFEPAQ-II EXFOR database is used in the visualisation described below, but to select or view the original EXFOR data it is necessary to have access to the EXFOR CD-ROMs. The correct CD-ROM must be present on the disk shown in the EXFOR disk text box in the Settings window (Figure 1). SAFEPAQ-II will warn the user (Figure 44) if the wrong CD-ROM is present in the drive; load the correct CD-ROM before clicking the OK button. Note that it is necessary to physically put the correct disk in the drive before clicking the OK button or SAFEPAQ-II will crash.

Figure 44. Warning that incorrect CD-ROM present.

Note that an updated version of the CD-ROMs has been provided by the NEA Data Bank. There are some differences in the format, and if the new version is used then the Original EXFOR CD check box on the Settings window (Figure 1) must be cleared. CDs containing EXFOR data for deuteron- and proton-induced reactions are available and must be used if the incoming particle is not a neutron.

The sources of data for a particular reaction can be viewed by clicking on EXFOR|EXFOR sources … or the eighth toolbar button to display the EXFOR sources window shown in Figure 45. A target nuclide is entered (Note that no isomeric targets are present in EXFOR), and a reaction selected from the dropdown list. Clicking the Sources button will display information on the available sources. The year of the experiment is given in the first column, '#' indicates that the data have already been selected in the EXFOR database. Under the Type column are a series of codes defined in the EXFOR documentation, but in addition, if the final state is given in the file then the symbols '->g', '->m' or '->n' are used to indicate g, m, n states respectively. The Lab codes, energies and the number of points are also shown. Selecting a particular source causes a ToolTip to be displayed which shows the Full Access number e.g. 40306.002 of the entry, this is a number that can be useful if the particular data file is required on the CD-ROM.

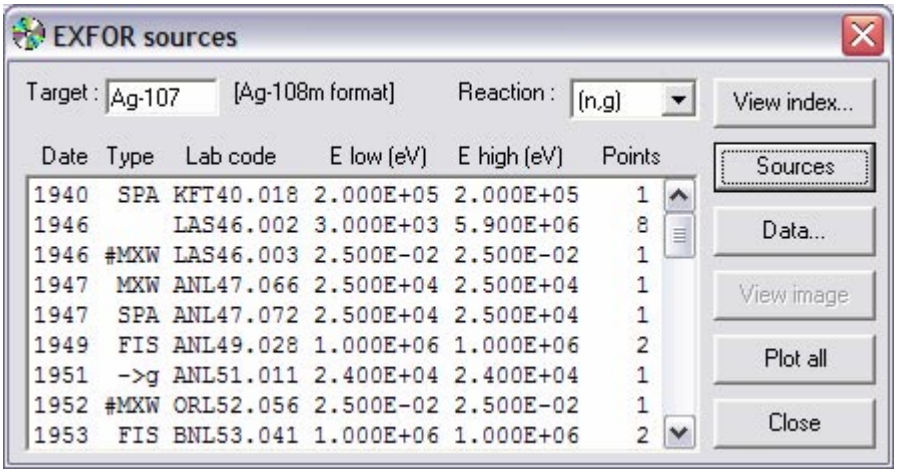


Figure 45. The EXFOR sources window.

It is possible to view the complete EXFOR index file for this nuclide by clicking the View index… button which displays the EXFOR index window shown in Figure 46. Note that if the columns do not line up correctly then adjust the value in the EXFOR index width text box in the Settings window (Figure 1).

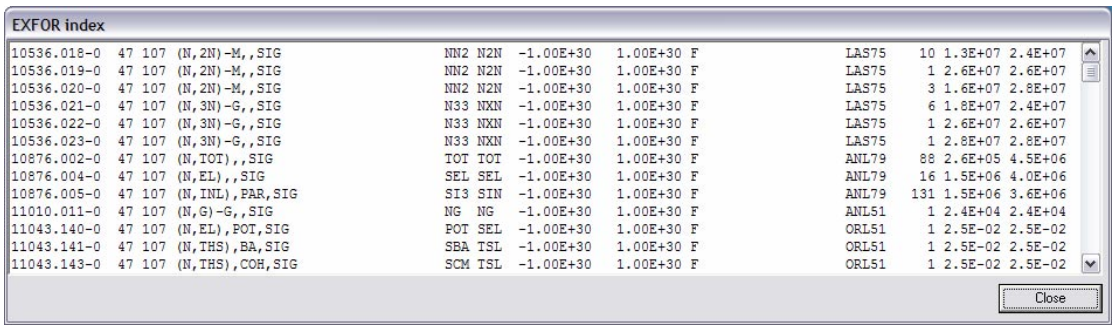


Figure 46. The EXFOR index window.

Selecting a particular source in Figure 45 enables a detailed view of the data by clicking the Data… button which displays the EXFOR data window shown in Figure 47 (the reaction name is placed in the title bar of the window). This displays information about the experiment (authors, institute, title of paper, reference and the neutron monitor), information on the daughter state (this is taken from the *DecayData* table in Parameter, not from anything stored in the EXFOR file) and the data points. In some cases the file specifies that a particular daughter state was measured, in this case the Final state can be selected from the available radio buttons. The original EXFOR file can be viewed by clicking the View file… button which displays the EXFOR file window shown in Figure 48. This is sometimes necessary to check on the final state or other details.

Note that in the Final state group the expected g, m, n and Total options are available. There is an additional entry Mixed,

which should be selected if the data points in the grid refer to different final states (as indicated in the FS column). If Mixed is selected then when the data are saved, these are stored in several entries with the correct final states.

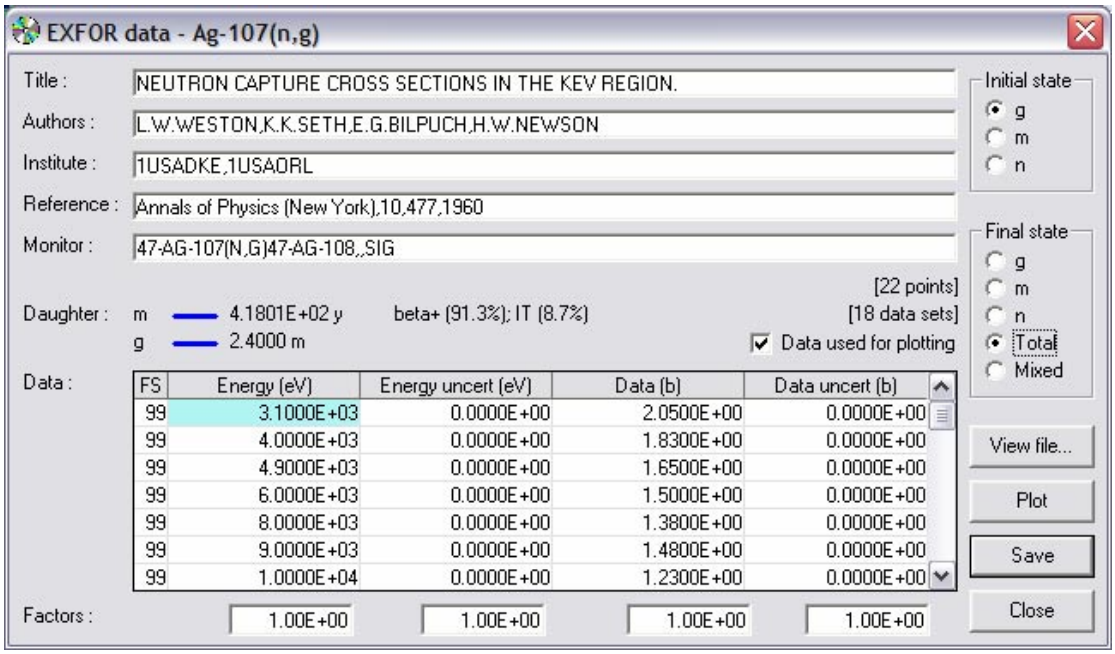


Figure 47. The EXFOR data window for a particular reaction.

For mixed cases it is possible that the FS entries shown in the grid are incorrect. If so then use the keys `0`, `1` or `9` (on the keyboard) to edit the entry. This information is saved correctly in the EXFOR database. However, when the data source is selected again the (incorrect) information from the CD-ROM is displayed in the grid.

Select a series of rows in the grid; pressing `Ctrl+C` copies the energy and cross section data to the clipboard, pressing `Ctrl+S` copies the energy and cross section data to a new scrap file with name `NuclideReaction_EXFOR` (see page 54 for more details of scrap files). These keyboard short cuts are displayed in a ToolTip if the cursor is hovered over the data grid.

By default the Reference information is expanded to make it more readable than the codes used in the EXFOR files. If there is an error caused by a reference not being correctly handled, then it is possible to switch off the expansion process. This is done by clearing the Expand EXFOR refs check box in the Settings window (Figure 1).

The number of points in the data set and the number of data sets for the reaction already selected are shown above the data grid. In some cases incorrect data are present on the EXFOR CD. This is typically due to cross sections or energies having

incorrect units. Provision is made to store factors for each entry that correct the error.

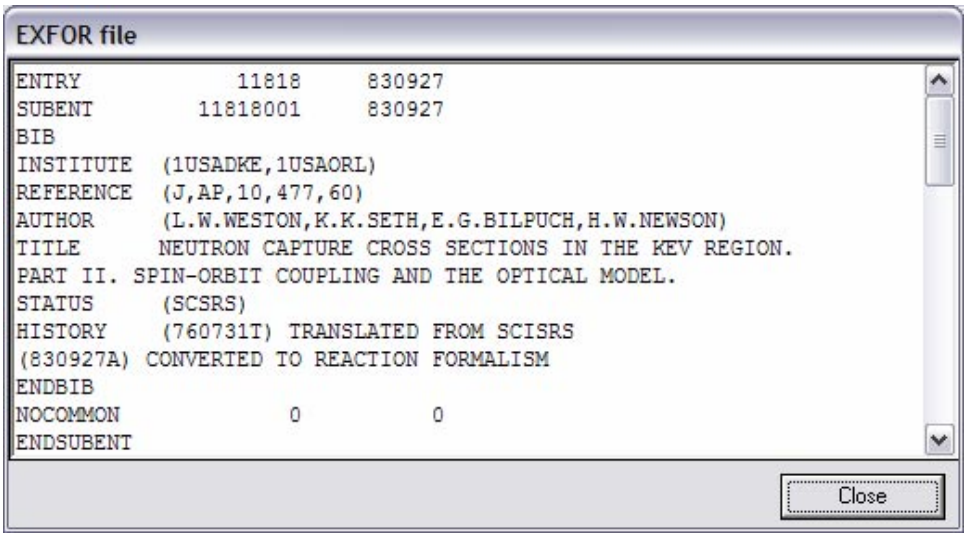


Figure 48. The EXFOR file window.

If after viewing it is decided that the data set is required then the Data used for plotting option should be checked and the Save button clicked. Depending on the reaction type there are various options when saving the data.

If the selected reaction is (n,x) then the dialog shown in Figure 49 is displayed. One of the radio buttons should be selected and the OK button clicked. The original EXFOR data will be saved as data for the reaction specified.

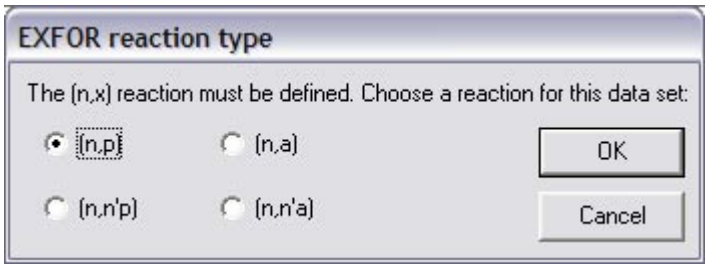


Figure 49. The EXFOR reaction type window for (n,x).

If the selected reaction is (n,n′p) or (n,d) then the dialog shown in Figure 50 is displayed. One of the radio buttons should be selected and the OK button clicked. The original EXFOR data will be saved as data for the reaction specified.

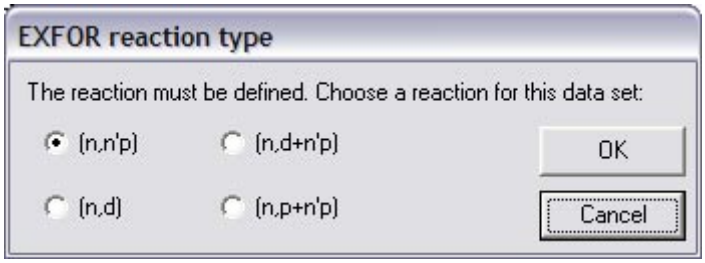


Figure 50. The EXFOR reaction type window for (n,d).

If the selected reaction is (n,n′d) or (n,t) then the dialog shown in Figure 51 is displayed. One of the radio buttons should be selected and the OK button clicked. The original EXFOR data will be saved as data for the reaction specified.

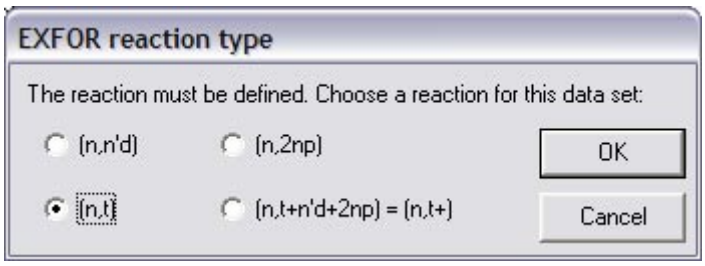


Figure 51. The EXFOR reaction type window for (n,t).

If the selected reaction is (n,h) then the dialog shown in Figure 52 is displayed. One of the radio buttons should be selected and the OK button clicked. The original EXFOR data will be saved as data for the reaction specified.

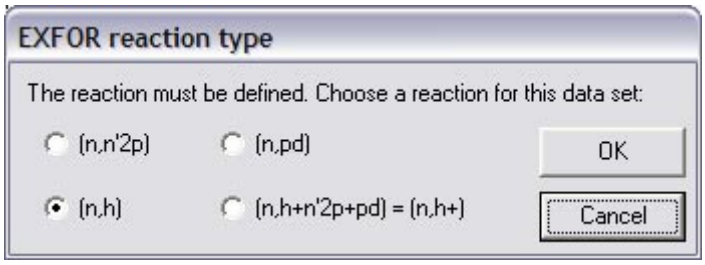


Figure 52. The EXFOR reaction type window for (n,h).

If the selected reaction is (n,α) then the dialog shown in Figure 53 is displayed. One of the radio buttons should be selected and the OK button clicked. The original EXFOR data will be saved as data for the reaction specified.

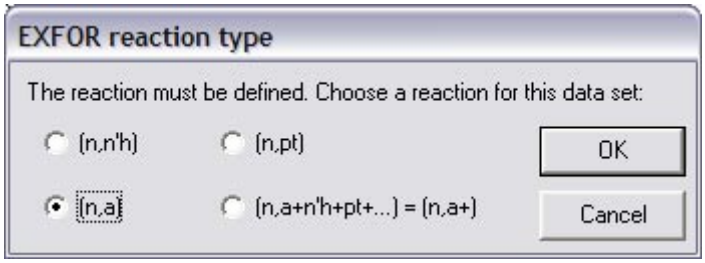


Figure 53. The EXFOR reaction type window for (n,α).

If the selected reaction is (n,n′α) then the dialog shown in Figure 54 is displayed. One of the radio buttons should be selected and the OK button clicked. The original EXFOR data will be saved as data for the reaction specified.

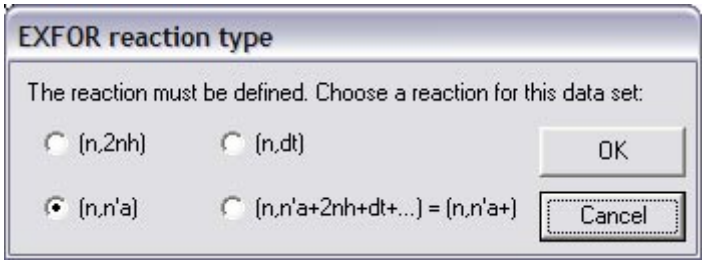


Figure 54. The EXFOR reaction type window for (n,n′α).

Note that if a summed reaction is chosen in Figure 50 - Figure 54 then the data are saved as a reaction with with an MT>200. However, they will be displayed on plots of reactions of both the summed and the base reaction. For example if data are saved for reaction type (n,α+), then on plots of both (n,α) and (n,α+) the saved EXFOR data will be displayed.

Clicking on the Plot button in Figure 47 displays the EXFOR plot window shown in Figure 55.

Figure 55 shows the data points for the selected data source. There are no options for changing axes types or scales, and it is designed just to enable a ‘quick look’ at the data. However, the graph can be printed to the default printer or copied to the clipboard by selecting the File|Print or Edit|Copy menu items.

Returning to Figure 45, it is possible to plot all the data sets that have been selected and saved in the EXFOR database by clicking the Plot all button. This displays the EXFOR master plot window shown in Figure 56. It is possible to change axes types, but the window is designed just to enable a ‘quick look’ at the data. By default the data are plotted with Lin/Lin axes, but by clicking on the Options|Log/Log axes menu item the graph is replotted with Log/Log axes. Clicking the Options|Lin/Lin axes menu item replots the graph with Lin/Lin axes. The graph can be printed to the default printer or

copied to the clipboard by selecting the File|Print or Edit|Copy menu items respectively. Note that the systematics values (at 14.5 MeV and 30 keV) are also shown if available.

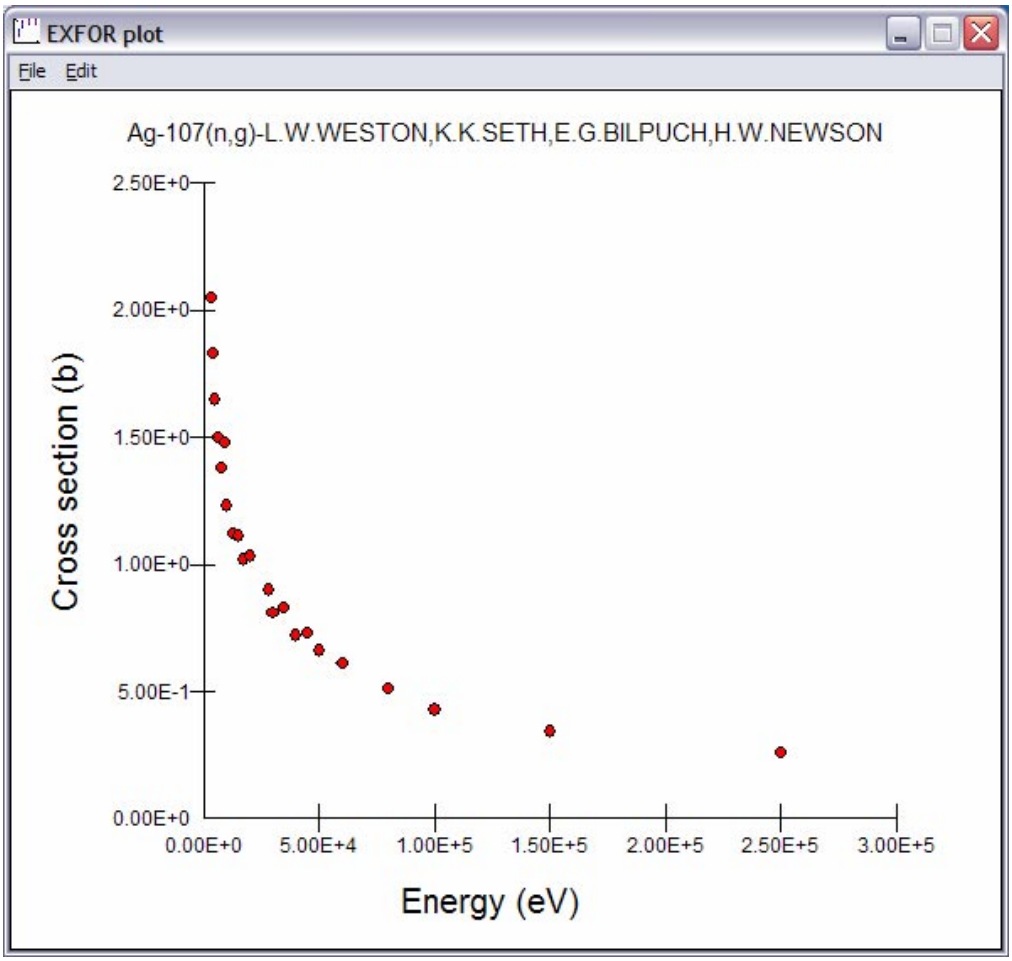


Figure 55. The EXFOR plot window.

An additional menu item, File|Save image, is available to save the current master plot to disk as an image (placeable Windows metafile format, `*.wmf`). This has the advantage that the particular image of the set of selected EXFOR sorces can be viewed later, even if the selected set has subsequently been altered. The image can be viewed by clicking the View image button on Figure 45, which displays the EXFOR image window shown in Figure 57. Note that this button will only be enabled if there is an available image for the reaction. All images are saved in the folder `graphs` shown in the Graphs folder text box on the Source database disk specified in the Settings window (Figure 1). A further use of images to construct a book is described later.

Experimental data that are too recent to be present on the EXFOR CD-ROMs may be available from other sources. If these are to be plotted then it is necessary to save them as Private EXFOR data. The menu item, EXFOR|Add Private

data… displays the Add Private data window shown in Figure 58. Enter the target in the first text box, select a reaction from the dropdown listbox and enter a lab code (use the standard EXFOR codes with the last two digits of the date; the codes can be obtained from the EXFOR lab codes window). Next select from one of the standard references (see Figure 40), enter the paper title and the authors in the next two text boxes, select the final state radio button and then select the file where the cross section data points are held. The data must be available in a standard `x4s` file (see start of this section). Clicking the Add button will put the data into the EXFOR database in two tables, *Private Reaction* and *Private cross section*. In cases where private data are added incorrectly it is possible to remove it by selecting the EXFOR|Delete Private data… menu item which displays the Delete Private EXFOR window shown in Figure 59. Select a reaction and click the Delete button to remove it. Note that if the data have already been stored in the EXFOR database, then a warning dialog is displayed stating that it is impossible to remove the data.

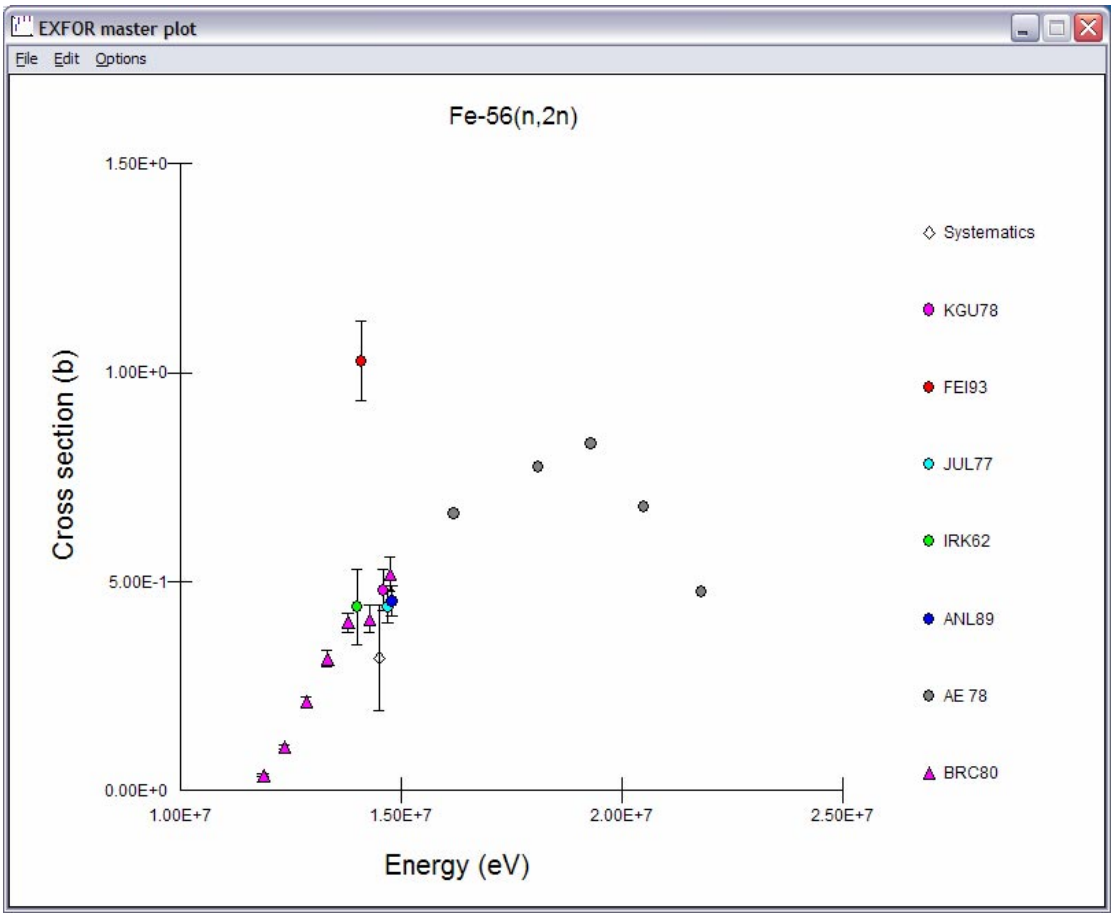


Figure 56. The EXFOR master plot window.

The EXFOR lab codes can be viewed by clicking the EXFOR|EXFOR lab codes … menu item that displays the EXFOR lab codes window shown in Figure 60. Select the

required country and the available lab codes and details are displayed in the grid.

When the EXFOR sources window (Figure 45) is opened, any private sources available for the selected reaction are appended to the end of the standard EXFOR sources. Note that if the data are stored in the SAFEPAQ-II EXFOR database then the symbol "&" is used rather than "#". Private data are not shown in the EXFOR index window (Figure 46). Clicking the Data... button in Figure 45 when a private source is selected displays the EXFOR data window shown in Figure 47. The private data are displayed as normal (but note that the View file... button is disabled). If the data are required to be stored in the SAFEPAQ-II EXFOR database then check the Data used for plotting option and click the Save button. The private data are displayed in plots (Figure 55 and Figure 56) in the same way as the standard EXFOR data.

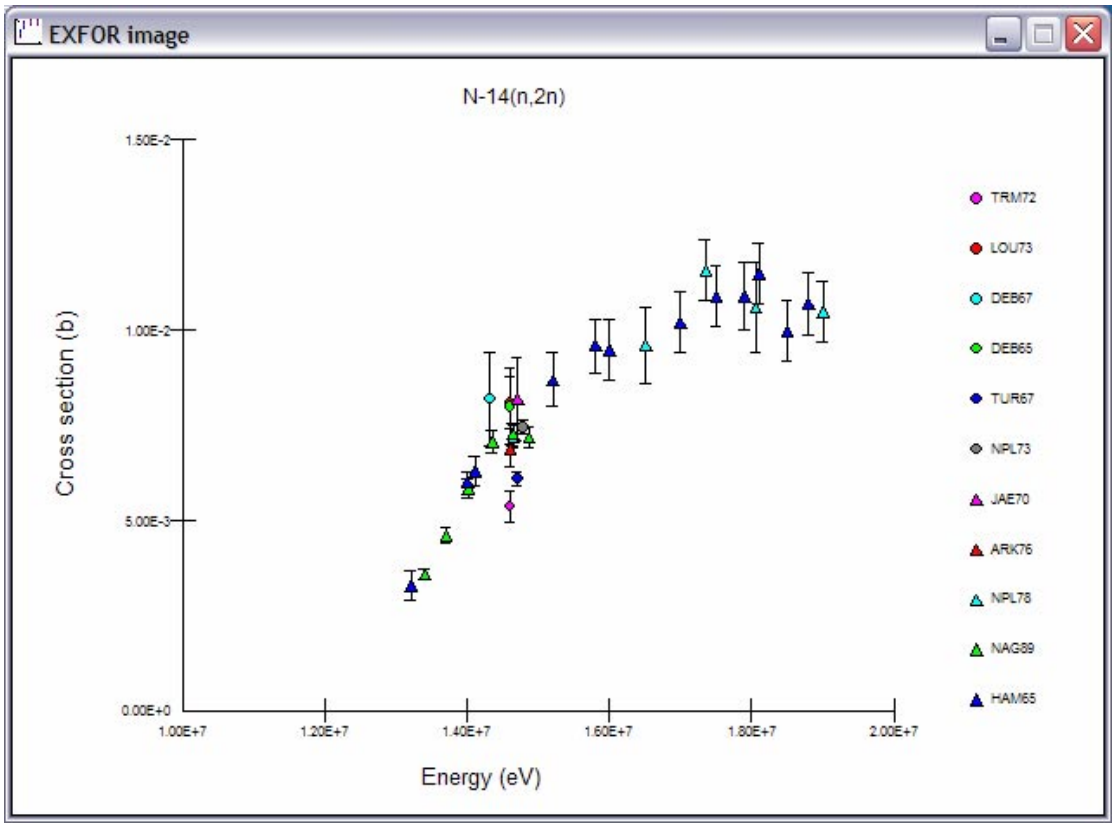


Figure 57. The EXFOR image window.

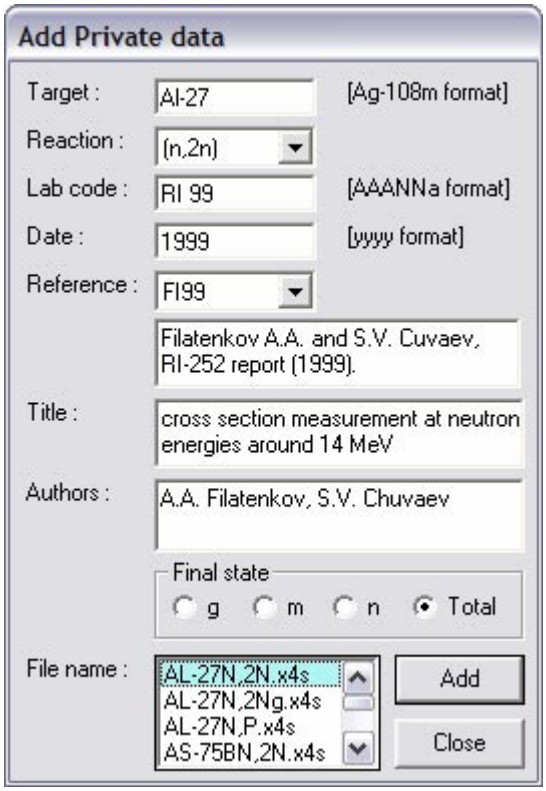


Figure 58. The Add Private data window.

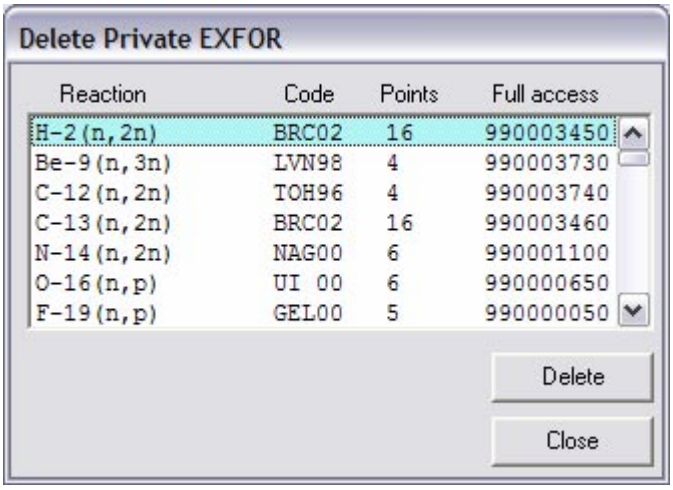


Figure 59. The Delete Private EXFOR window.

Returning to the main SAFEPAQ-II window, Figure 2. Clicking the second item on the EXFOR menu, List EXFOR entries… displays the List EXFOR entries window shown in Figure 61. Select a reaction type from the dropdown list and click the Get entries button to display all the reactions stored for the given reaction type with the Final state (FS = g, m, n or blank for a total) and the Lab code. The number of entries is shown. By default the standard EXFOR entries are displayed, but by clicking the Private option in the Type group, the Private EXFOR entries can be listed.

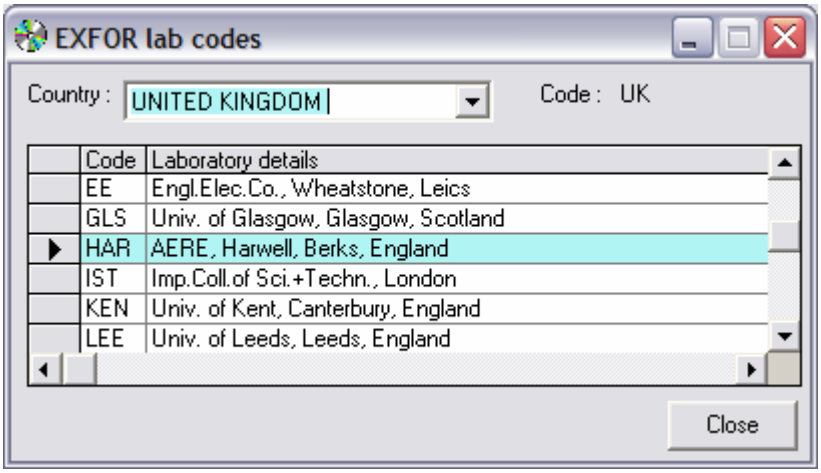

EXFOR lab codes
Country : UNITED KINGDOM
Code : UK
Code Laboratory details
EE Engl.Elec.Co., Wheatstone, Leics
GLS Univ. of Glasgow, Glasgow, Scotland
HAR AERE, Harwell, Berks, England
IST Imp.Coll.of Sci.+Techn., London
KEN Univ. of Kent, Canterbury, England
LEE Univ. of Leeds, Leeds, England
Close

Figure 60. The EXFOR lab codes window.

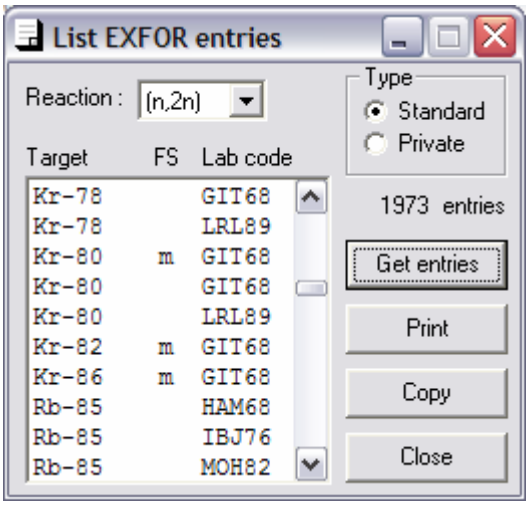


Figure 61. The List EXFOR entries window.

Clicking the Copy button copies all the entries to the clipboard. The list can be printed to the default printer by clicking the Print button.

Clicking on the third item on the EXFOR menu, Assemble book… or the ninth toolbar button, displays the Assemble book window shown in Figure 62.

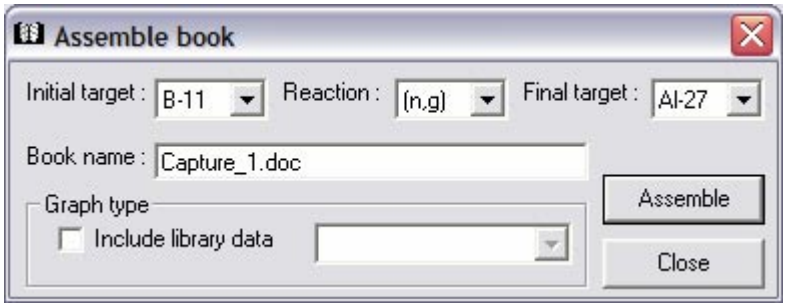


Figure 62. The Assemble book window.

This window allows a series of images to be plotted in a Word document (a book) and then printed out for further study. Choose the range of graphs by selecting the intial and final targets and the reaction type in the dropdown list boxes. Give a name for the book (.doc is always present in the text box) and then click on the Assemble button. This will produce the Word file containing all the images for the specified targets and reaction with two plots per page. As described above, the EXFOR images are used. It is also possible to produce a book of images that contain EXFOR data and points from one of the standard data libraries. These images are described later (page 47), but if they are available then a book can be assembled using them if the Include library data option is checked and the required Source ID is selected in the dropdown list box.

Visualisation

The ability to visualise cross section data in the various source libraries and in the SAFEPAQ-II databases is essential in the evaluation and selection of data for inclusion in EAF. Comprehensive tools are available in SAFEPAQ-II to accomplish this. Clicking on the Visualisation|Targets and sources… menu item or the sixth toolbar button displays the Targets and sources window shown in Figure 63.

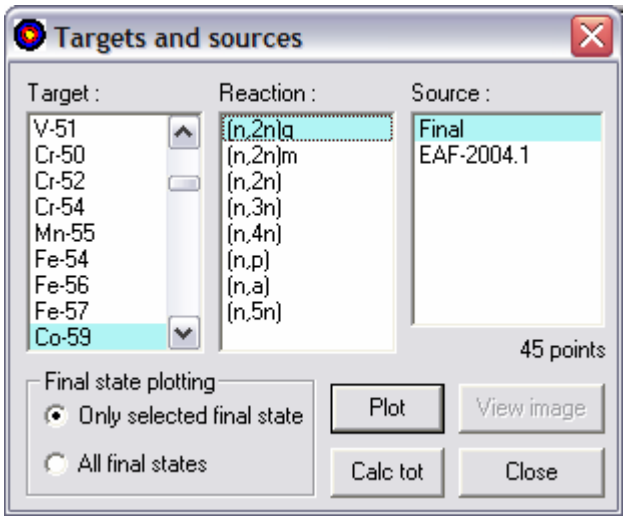


Figure 63. The Targets and sources window.

This window displays the reactions present in the Cache database. Cache is one of the SAFEPAQ-II databases and provides a store where data from any of the source libraries or the SAFEPAQ-II databases (Master, Final or Test) can be placed for comparison and plotting. Unlike the other databases where data from only a single source for any reaction can be present, Cache can contain multiple copies of data for the same reaction from a variety of sources. The Target nuclides present

in Cache are shown in the first list box, selecting a target displays the reactions for that target in the second list box and selecting a reaction shows the sources of the data in the third list box. The number of data points in the data set is shown for the reaction from the selected source. Selecting the Only selected final state radio button means that in cases where there are several isomeric states then only the selected final state (in Figure 63 this would be the g state) will be plotted. If this radio button is selected, then it is possible to plot data from all or any of the Sources. This is done by clicking on the first source with the mouse and then clicking on the last source with the `Shift` key pressed, or by clicking on each required source with the `Control` key pressed. Note that if several sources are selected then the number of points of the first selected is shown.

Note that when opening this window the target used for plotting when the window was previously closed will be selected. This feature introduced from EASY-2005 saves time when plotting data.

Clicking the Plot button will display the Data visualisation window shown in Figure 64. This shows data for the Co-59(n,2n) reaction for all final states (the All final states radio button was clicked in Figure 63). Because the total cross section for the g and m states has been calculated (see page 59) three curves are present in Figure 64. In addition to the curves, experimental data for the reaction stored in the Parameter database are plotted as red triangles. The key for the curves is at the bottom of the plot. The Data visualisation window presents many options for the user, and is probably the most complicated in the whole application. It contains a menu bar, a toolbar and a status bar. The latter is used to present information about a data point on the graph selected by clicking with the mouse.

In Figure 64 one of the red data points has been clicked, the status bar shows that it is Experimental data, the number of the data point, its energy, cross section and its final state (‘g’, ‘m’, ‘n’ or ‘T’ for total cross section).

A shortcut method of ploting the data is to double click the required data source in the Targets and sources window (Figure 63). Note that if a library with data > 20 MeV is being used then the x-axis in Figure 64 extends up to 60 MeV, otherwise the limit is 20 MeV.

Clicking the Edit|Copy menu item or the first toolbar button copies the current plot to the clipboard. Clicking the File|Print menu item or the second toolbar button prints the current plot.

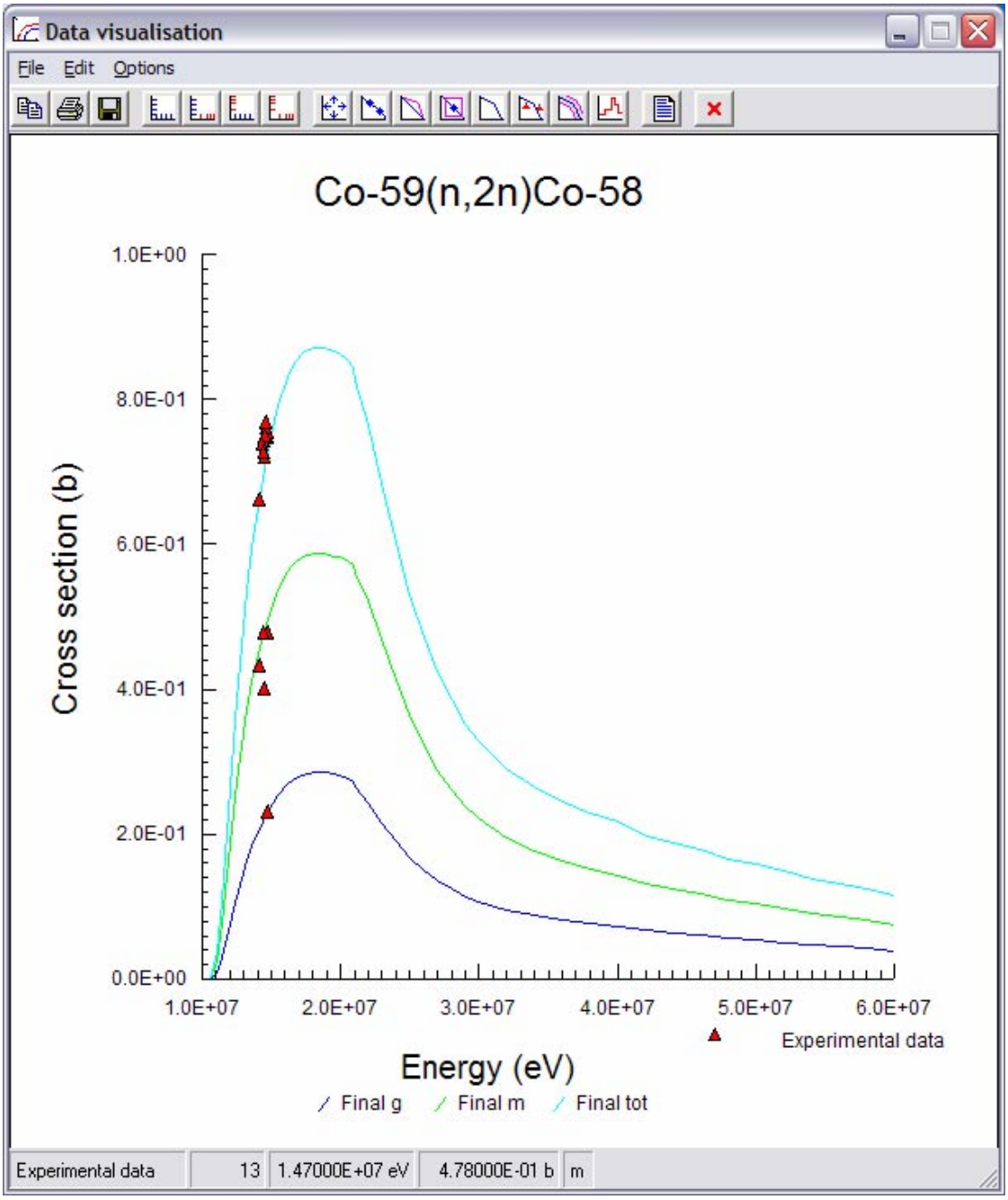


Figure 64. The Data visualisation window.

Clicking the File|Save image menu item or the third toolbar button saves the current plot as an image, this can then be written to a Word file as a book as described on page 44. Clicking the Options|x/y axes menu item displays a submenu that shows the four axes combinations (fourth - seventh toolbar buttons) that can be used to plot the data. Clicking the Options|x/y ranges menu item or the eigth toolbar button displays the x/y ranges window shown in Figure 65. This shows the current minimum and maximum values on the x and y axes and allows new values to be entered. The previous values are stored and can be recalled by clicking the Last

button. This saves time if the same changes are required on a series of graphs. Clicking the Apply button makes the changes. The window remains open until closed by clicking the Close button.

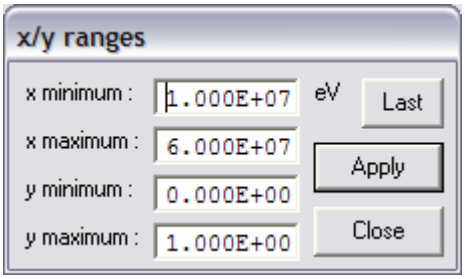


Figure 65. The x/y ranges window.

Checking the Options|Legend menu item displays a submenu that shows the two positions of the EXFOR legend on the plot (Right or Left). Changing this can be useful if the legend overlaps the data points. Checking the Options|Show symbols for data points menu item or the ninth toolbar button plots the data points that make up each curve. Checking the Options|Show interpolated values menu item or the tenth toolbar button shows the position of interpolated data between the selected data points (determined by the interpolation law between the points). To use this it is necessary to first click this and then click the data selection tool and then select the points by dragging with the mouse.

Checking the Options|Data selection menu item or the eleventh toolbar button changes the cursor to a cross hair and enables points to be selected (click and drag the mouse to display a rubber band around the selected points). Checking the Overplot experimental menu item or the twelth toolbar button plots the experimental data points (note that clicking the toolbar actually stops the plotting of the data points – the graph is cleared). Checking the Options|Overplot EXFOR menu item or the thirteenth toolbar button removes the experimental data points and plots any available EXFOR data instead. Note that if the Options|Include exp with EXFOR menu item is checked then both the experimental data and EXFOR points will be displayed.

Checking the Options|Overplot uncertainty band menu item or the fourteenth toolbar button displays an uncertainty band (using the uncertainty values shown in Figure 35 and Figure 38) over the main curve. The error factors and the source of data are shown in the status bar. Note that this option will only work if a single final state and a single source are selected.

Clicking the Options|Overplot group data menu item displays a submenu that shows the twelve options for overplotting group data (No group data and the eleven group structures). One of these group structures can be selected in the

Settings window (Default group data type) as the group structure that is shown when the fifteenth toolbar button is clicked.

Checking the Options|Draw in black and white menu item means that graphs will be displayed on screen with the lines black but distinguished by various patterns. This is useful if graphs are copied to the clipboard for use in other documents that will not be printed in colour.

Checking the Options|Draw lines thick menu item means that graphs will be displayed on screen with the lines thick, making them more visible. This is useful if graphs are copied to the clipboard for use in other documents.

Checking the Options|Print lines thick menu item means that graphs will be printed with the lines thick, making them more visible. Clicking the Options|Redraw menu item replots the graph.

Checking the Options|2 dec. pl. on x-axis and Options|2 dec. pl. on y-axis menu items means that graphs will be displayed with the values on the axes having 2 decimal places rather than the default of 1. This is necessary if the range of the values is chosen to be small.

Clicking the Options|Reaction data window for menu item displays a submenu that shows the names of the various curves that are plotted (either final states or data sources). Clicking one of these will display the Reaction data window for the selected reaction shown in Figure 66. The Reaction data window for the first reaction can also be opened by clicking the sixteenth toolbar button.

Checking the Options|Reaction data warning menu item (checked by default) means that if data for a sum are to be displayed in the Reaction data window then a warning dialog with the message 'Unknown reaction (possibly a sum?)' is displayed prior to the window appearing. If this warning is not required then it can be removed by clearing the check on this menu item.

If EXFOR data are shown then clicking on a data point will give information about the selected point. If only the curves are plotted (preferrably with the data point symbols shown), then clicking on a point will give information about it (including the interpolation law in the final pane) in the status bar.

If the plotted curve is from Final and is not a summed reaction then clicking with the left button of the mouse on the status bar brings up a ToolTip showing the source of data.

If the plotted data have been produced by a Data merge modification (Mod type 13, see Table 2 for details) then there

may be a discontinuity in the data that requires a further modification (Mod type 4) to scale the high energy data so as to end up with continuous data. To calculate this factor the following procedure should be used. Show the symbols for the data points and click on the last point prior to the discontinuity. Note that if experimental data are plotted then it will be necessary to click the twelfth toolbar button to clear the experimental points. The information for the selected point is shown in the status bar. Using the left mouse button double click on the status bar to bring up a ToolTip showing the factor by which it is necessary to scale the high energy data to achieve continuity. This works by using extrapolation (using the correct law) on the selected and the previous point to predicted the new value at the point above the selected one.

One restriction on the above calculation of factors must be noted. If the number of data point for a reaction is very large (> 32,767) then the data are thinned prior to plotting (only every other point is plotted). For such reactions the data source in the status bar is followed by ' – thinned', and because it may not be possible to click on the actual point before the discontinuity, the ability to calculate factors is disabled for reactions with thinned data.

The Reaction data window shows the source of data in the title bar, and the reaction above the data grid. Note that if data from Final, Master or Test are used then the original data source is also shown in < > brackets. In addition, if there are *p* pre-modifications and *m* modifications, then these are shown as '+p,m' following the original data source. The number of data points is shown to the right of the reaction. The point number, energy and cross section are shown in the grid. The various interpolation law ranges are shown in the lower list box, and if points are selected in the grid then these are also indicated in the upper text boxes. The selection of data points is linked to the Visualisation data window, if points are selected there, and the Reaction data window is open then the points in the grid are also shown selected. The selected data can be copied to the clipboard by clicking the Copy button. The entire grid can be printed by clicking the Print button.

The reaction number used in the databases to identify the reaction is sometimes required. This can be found (so long as the reaction exists in Parameter) by clicking on the reaction name at the top left of the window, a ToolTip showing the reaction number is displayed when the cursor hovers over the reaction name.

The energy and cross section values in the grid are displayed to six decimal places. The database holds these values to higher precision, and especially if changing the value of a cross section

at an energy point, it is necessary to know the values more precisely. This is possible by selecting a single row and holding the cursor over the grid, a ToolTip is shown with the values to twelve decimal places.

Some data sets contain many points, and because of a limit on the number of rows in the data grid and also to speed up loading the data, it is necessary to split a large data set into 'pages'. Each page contains a maximum of 10,000 data points, and if paging is necessary then the < and > buttons are enabled. These display the next (>) and previous (<) page of data as appropriate.

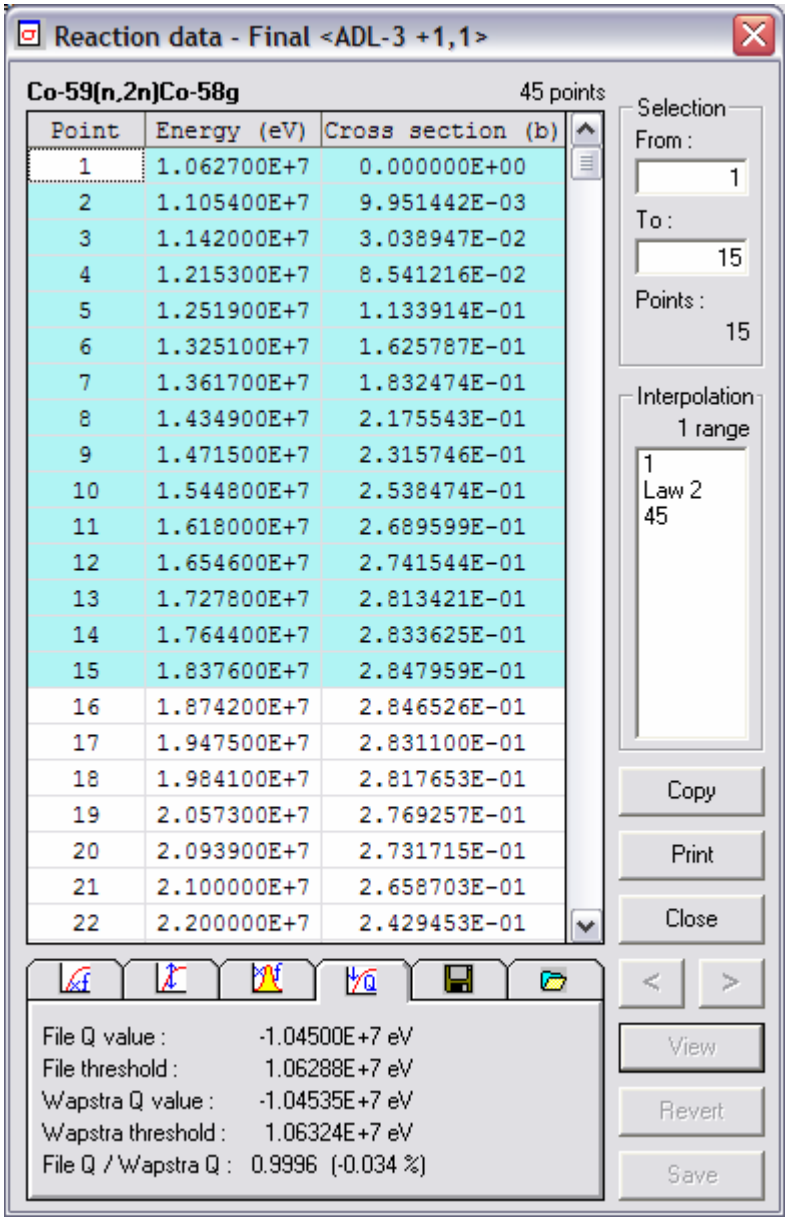


Figure 66. The Reaction data window.

At the bottom of the Reaction data window are six tabs. By default the fourth is shown when the window opens. This

shows the *Q*-value and threshold for the file and those from the Wapstra mass table. The ratio gives a good indication as to whether the *Q*-value is correct in the file. The Save tab is also active for any data source, but if the source of the reaction data is the Test database (but not for any other source), then the other four tabs become active. The five tabs other than the fourth one shown in Figure 66 are shown in Figure 67 - Figure 71.

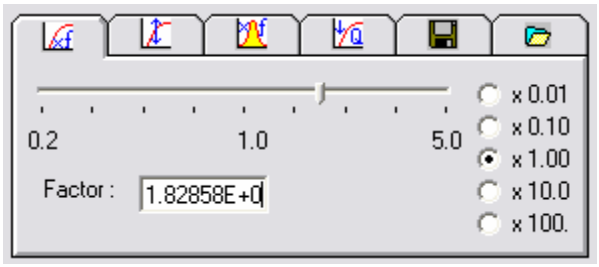


Figure 67. The Scale tab of the Reaction data window.

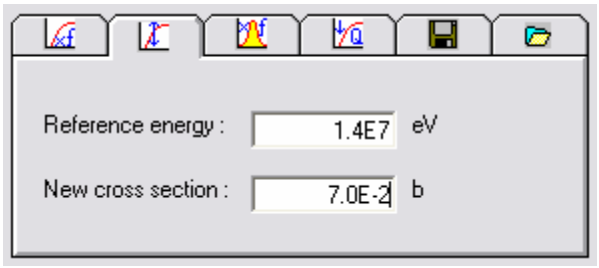


Figure 68. The Renormalise tab of the Reaction data window.

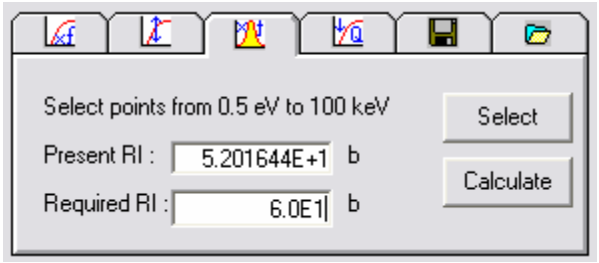


Figure 69. The Resonance integral tab of the Reaction data window.

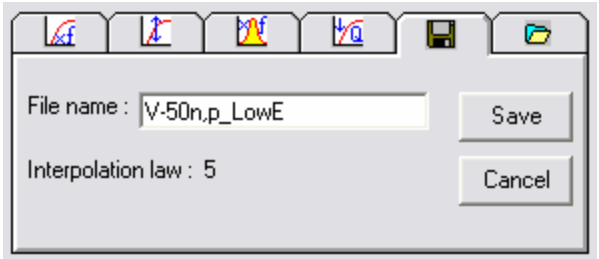


Figure 70. The Save tab of the Reaction data window.

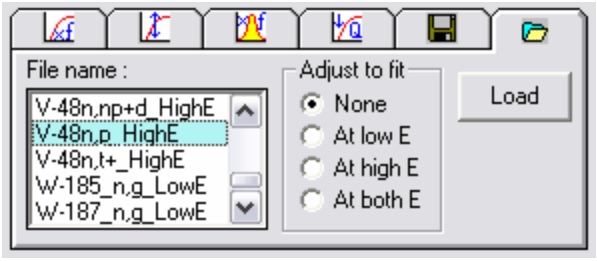


Figure 71. The Load tab of the Reaction data window.

The Scale tab (Figure 67) enables a scale factor to be chosen by choosing a range radio button and dragging the slider. The resultant factor is shown in the text box. Select the data points that this modification should apply to and the View button becomes enabled. Clicking this will plot the modified data. If this is not correct then clicking the Revert button will plot the original data. If the change is useful, then it can be saved as a modification for the reaction by clicking the Save button.

The Renormalise tab (Figure 68) enables a new cross section at a reference energy to be entered in the text boxes. Select the data points that this modification should apply to and the View button becomes enabled. Clicking this will plot the modified data. If this is not correct then clicking the Revert button will plot the original data. If the change is useful, then it can be saved as a modification for the reaction by clicking the Save button.

The Resonance integral tab (Figure 69) contains two buttons. Clicking Select will select data points in the range 0.5 eV – 100 keV. Clicking Calculate will calculate the resonance integral for the reaction and show the result in the first text box (Note that this text box cannot be edited). Enter the new resonance integral value in the second text box. Clicking the View button will plot the modified data. If this is not correct then clicking the Revert button will plot the original data. If the change is useful, then it can be saved as a modification for the reaction by clicking the Save button.

It is possible to save the selected data points as a 'scrap' of data. This is saved with the file name specified in the text box on the Save tab (Figure 70) in the folder `scraps` shown in the Scrap folder text box on the Source database disk specified in the Settings window (Figure 1). The interpolation law applying to the selected points is also saved. Note that it is not possible to have a data scrap with more than one interpolation law. This tab should be clicked and then the points required selected. A file name will be suggested in the text box based on the current reaction (in Figure 70 this was `V-50n,p_` which can

then be customised as required. Clicking the Save button on the tab writes the scrap to the file.

Data scraps can be merged with the current reaction data (if these are from Test) using the Load tab (Figure 71). The scraps can either have been generated using the Save tab or by using the Scrap editor described below. The available scraps are shown in the list box, select one of these and then click one of the radio buttons in the Adjust to fit group. If None is selected then the scrap data replace data in that range for the current reaction. If At low E is selected then the scrap data are scaled so that they have the same value as the current data at the low energy point. If At high E is selected then the scrap data are scaled so that they have the same value as the current data at the high energy point. If At both E is selected then the scrap data are scaled so that they have the same value as the current data at both the low and high energy points. This is done by scaling by a factor that varies linearly with energy between the given factors at the low and high energies.

Data scraps were described above. Although it is useful to be able to extract these from an existing file, it may be necessary to create one from scratch for a particular reaction. This can be done using the Scrap editor window shown in Figure 72. This is displayed by clicking on Visualisation|Scrap editor… or the seventh toolbar button.

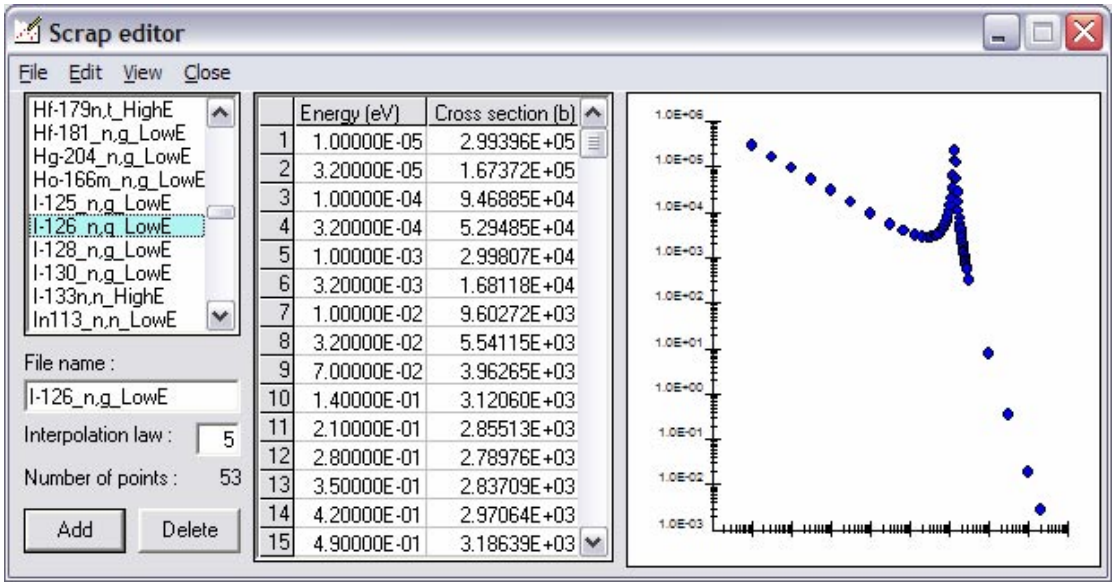


Figure 72. The Scrap editor window.

Existing data scraps can be viewed by selecting the file name in the list box and clicking the File|Load menu item (a shortcut is to double click the file name). This shows the energy and cross section of the points in the data grid, the interpolation law in the text box and the number of points. A small graph of the data

appears on the right of the data grid. Data in the grid can be edited by selecting a number and typing. Note that typing will overwrite the existing value, if you require to edit, then click on the number and press the Space key.

A new data point can be added by selecting the data point which you require to have the new point added after and clicking the Add button. The number of points increases and new values can be entered. To remove a data point, select the point and click the Delete button. The new scrap can be saved, either overwriting the existing file, or by entering a new name in the text box. A new scrap can be constructed by clicking File|New and entering data. The appearance of the graph can be altered, checking the View|Lin/Lin axes menu item will plot using both axes linear and checking the View|Log/Log axes menu item will plot using both axes logarithmic. The data points can be joined by checking the View|Show lines menu item. The selected items in the data grid can be copied to the clipboard by clicking the Edit|Copy menu item. The entire scrap file can be printed by clicking the File|Print menu item. Closing the window (either by clicking the File|Close or the the Close menu items) without saving the changed data displays a confirmation dialog that gives the chance to save the file.

An example of the use of data scraps is the calculation of the capture and fission cross sections in the energy range 1 10^{-5} eV to the end of the resolved resonance region (E_H). This can be done using the Single Resonance Approximation (SRA) which is described in Appendix 5. To generate the data scrap for a capture reaction click on the Visualisation|Create (n,g) scrap using SRA… menu item which displays the Create (n,g) scrap using SRA window shown in Figure 73. Enter the target in the first text box, then click on one of the other text boxes. As much information as possible is then filled in the boxes automatically from the Parameter database, typically it will only be necessary to enter a Resonance energy if an experimental thermal cross section and Resonance integral exist. Choose the final state and then click the Calculate button. This writes the data scrap with the given file name and calculates the SRA Resonance integral. If the Upper energy (E_H) value is less than the normal upper limit for a RI calculation (100 keV) then a red warning symbol is shown to the right of the ratio. A ToolTip explains this symbol further.

Various values of the resonance energy can be tried in order to achieve a calculated RI close to the experimental value. The data scrape can be viewed and edited from within the Scrap editor window (Figure 72) as described above.

To generate a data scrap for a fission reaction click on the Visualisation|Create (n,f) scrap using SRA… menu item which displays the Create (n,f) scrap using SRA window similar to that shown in Figure 73. The only difference is that it is not necessary to select a final state.

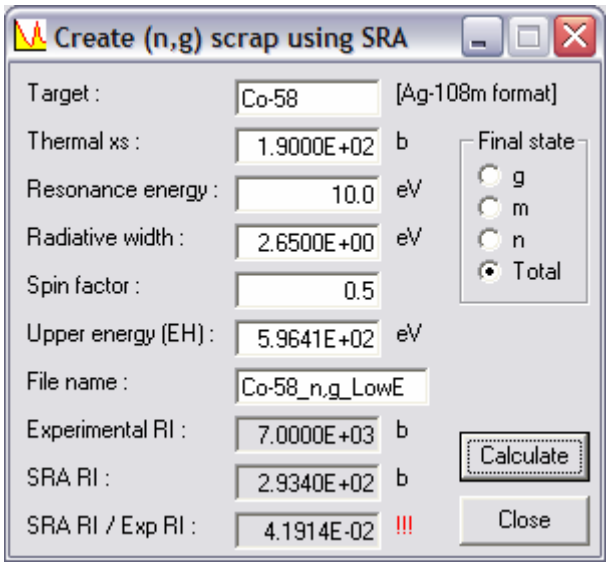


Figure 73. The Create (n,g) scrap using SRA window.

In the Targets and sources window (Figure 63) it is possible to visualise branching ratio data. This is done by clicking on the Plot BR button. Note that the caption on this button and whether it is enabled vary depending on the reaction selected. In most of the libraries used by SAFEPAQ-II, reactions that have more than one final state only have reactions to the separate final states but not the sum present. Cache is able to also contain the sum, but before a branching ratio can be plotted, it is necessary that the sum be calculated. If a reaction is selected with a final state of 0, 1 or 2 and the sum has not already been calculated then the button shows the caption Calc tot. Clicking this will form the sum of the data to the final states and store the total in Cache. Note that if all the final states have data 'on the same energy grid', then the calculation is fairly fast even with a large number of points. However, if the energy grid differs then interpolation is required to form the sum, and this can take some time.

Following the calculation an additional reaction will appear in the Reaction list box and the button caption will become Plot BR and the button will be enabled. Clicking on this button will display the Branching ratio visualisation window shown in Figure 74. This is similar to the Data visualisation window (Figure 64) but with a reduced set of options. There is no toolbar, but the status bar is used to display information on the points. In Figure 74 the lower of the red triangles has been clicked, information on it is shown in the status bar.

Clicking the File|Print menu item prints the plot to the current printer. Clicking the Edit|Copy menu item copies the plot to the clipboard. Clicking the Options|x/y axes menu item displays a submenu that shows the four axes combinations that can be used to plot the data. Checking the Options|Show symbols for data points menu item plots the data points that make up each curve. Checking the Overplot experimental menu item plots the experimental data points. If this is not checked then information on the curve data points can be shown in the status bar.

Note that if there are a large number of data points, then plotting the graph can take a significant time.

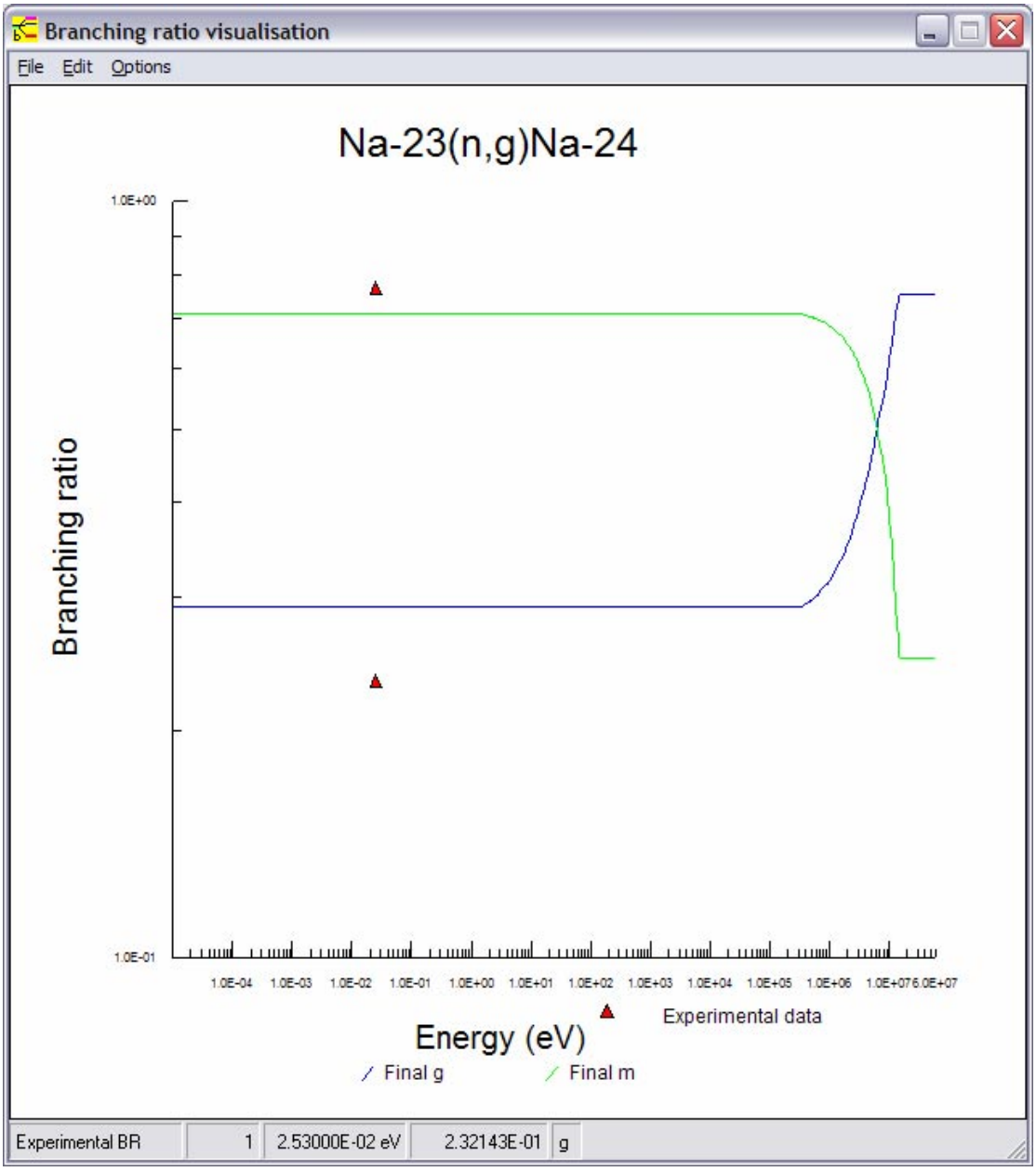
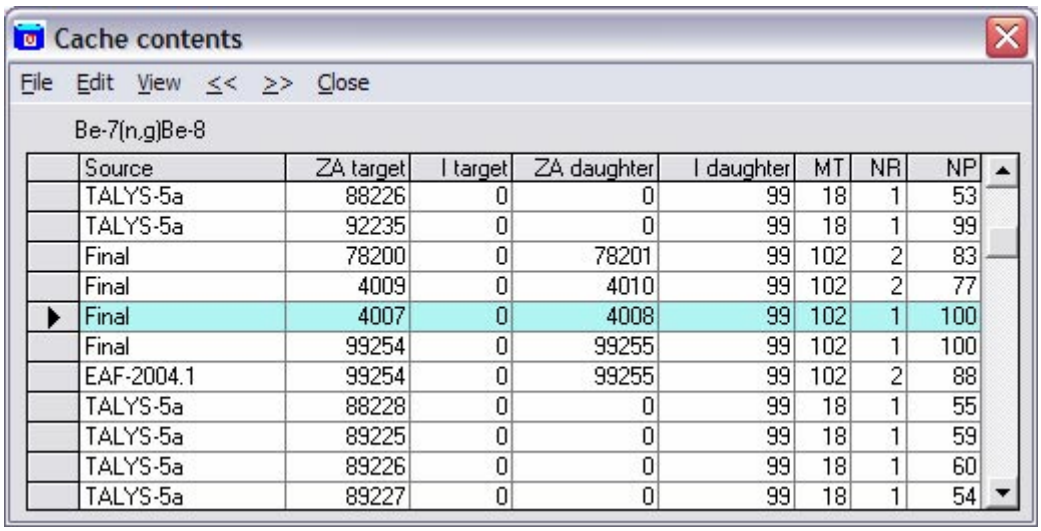


Figure 74. The Branching ratio visualisation window.

In the descriptions above the Cache database has been mentioned several times. The contents of the Cache can be viewed by clicking the File|Cache contents… menu item or the second toolbar button in the main window. This displays the Cache contents window shown in Figure 75. The data grid shows the reactions that are present, clicking to the left of the first column will select a reaction and display it in an easy to read format above the grid. The Source of the reaction is shown in the first column. The standard ZA and isomeric state values for the target and daughter are shown in the second to fifth columns. The ENDF MT reaction code is shown in column six, and the number of interpolation ranges (NR) and number of data points (NP) are shown in the final two columns.



Source	ZA target	I target	ZA daughter	I daughter	MT	NR	NP
TALYS-5a	88226	0	0	99	18	1	53
TALYS-5a	92235	0	0	99	18	1	99
Final	78200	0	78201	99	102	2	83
Final	4009	0	4010	99	102	2	77
Final	4007	0	4008	99	102	1	100
Final	99254	0	99255	99	102	1	100
EAF-2004.1	99254	0	99255	99	102	2	88
TALYS-5a	88228	0	0	99	18	1	55
TALYS-5a	89225	0	0	99	18	1	59
TALYS-5a	89226	0	0	99	18	1	60
TALYS-5a	89227	0	0	99	18	1	54

Figure 75. The Cache contents window.

Clicking the Edit|Find... menu item displays the Find window shown in Figure 76. Enter the required target nuclide and click the Find First button (or use the Enter key) to display this reaction in the Cache grid. Futher reactions with this target can be found by clicking the Find Next button (or use the Enter key). The window can be closed by clicking the Close button.

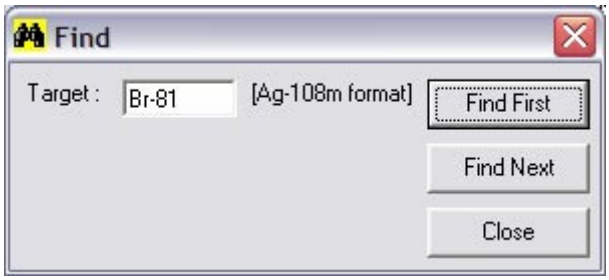


Figure 76. The Find window.

Clicking the View|Reaction data... menu item displays the Reaction data window (Figure 66) for the selected nuclide. Clicking the >> and << menu items moves to the end and

beginning of the Cache data respectively. A reaction can be removed from the Cache by clicking the Edit|Delete reaction menu item, the Cache can be emptied by clicking the Edit|Delete All menu item. Prior to the data being removed, the confirmation dialog shown in Figure 77 is displayed.

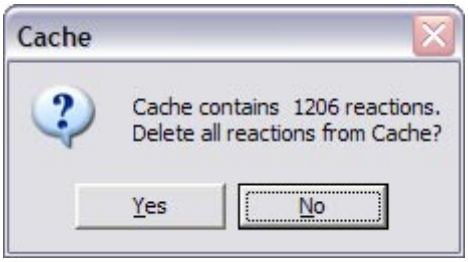


Figure 77. The confirmation dialog prior to emptying the Cache.

All the reactions for the selected target and source can be removed from the Cache by clicking the Edit|Delete all reactions for target and source menu item, no confirmation is necessary prior to removal. If summed reactions with MT>200 have been produced (see later), then these can be removed from the Cache by clicking the Edit|Delete all MT>200 sums for target and source menu item, no confirmation is necessary prior to removal.

It is possible to combine data in the Cache in several ways. Firstly, if a reaction has more than one final state, then the sum (I daughter = 99) can be formed by clicking the Edit|Add sum of isomeric cross sections menu item. Secondly, if more than one reaction from the same source form the same daughter, then these can be added by clicking the Edit|Add sum of cross sections for same daughter menu item. The exact meaning of this sum is actually more general then the cross section to the same daughter since particle production cross sections are also formed. The selected reaction must be (n,n′p), (n,d), (n,p), (n,t), (n,n′t), (n,h), (n,n′h), (n,α) or (n,n′α), and one of the sums (n,d+n′p), (n,t+n′d), (n,p+n′p), (n,t+n′t), (n,h+n′h) or (n,α+ n′α) is formed. Note that because of the first two sums it is not possible to produce (n,d+n′d), this must be done by using the next menu item. Also that these particle production sums contain only the first two terms of the more general sums, such as (n,xp), defined in Table 1.

At energies above 20 MeV many other summed reactions are important. In order to produce these all the reactions for a particular reaction and source should be copied to the Cache. See the option on the Data selection window (Figure 78) to copy all reactions to the Cache. Because many reactions are split and summed reactions are totals it is necessary to add all the split reactions together. Clicking the Add isomers for all

reactions for target menu item does this for the selected target. Clicking the Edit|Add cross sections to create all MT>200 sums menu item will produce as many summed cross sections as possible. The various possibilities and the definition of the summed reactions are shown in Table 1.

Table 1. Details of the summed reactions with MT>200.

MT	Reaction	Summed reactions
201	(n,n′p+d)	(n,n′p), (n,d)
202	(n,xn)	(n,2n), (x,3n), (x,4n), (x,5n), (x,6n), (x,7n), (x,8n)
203	(n,xp)	(n,p), (n,n′p), (n,2np), (n,3np), (n,pα)
204	(n,xd)	(n,d), (n,n′d), (n,2nd), (n,3nd), (n,dα)
205	(n,xt)	(n,t), (n,n′t), (n,2nt), (n,3nt), (n,tα)
206	(n,xh)	(n,h), (n,n′h), (n,2nh), (n,3nh), (n,ph)
207	(n,xα)	(n,α), (n,n′α), (n,2nα), (n,3nα), (n,pα)
208	(n,t+)	(n,t), (n,n′d), (n,2np)
209	(n,n′t+)	(n,n′t), (n,2nd), (n,3np)
210	(n,2nt+)	(n,2nt), (n,3nd), (n,4np)
211	(n,3nt+)	(n,3nt), (n,4nd), (n,5np)
212	(n,4nt+)	(n,4nt), (n,5nd), (n,6np)
213	(n,5nt+)	(n,5nt), (n,6nd), (n,7np)
214	(n,h+)	(n,h), (n,pd), (n,n′2p)
215	(n,α+)	(n,α), (n,n′h), (n,pt), (n,n′pd), (n,2n2p)
216	(n,n′α+)	(n,n′α), (n,2nh), (n,dt), (n,n′pt), (n,3n2p)
217	(n,2nα+)	(n,2nα), (n,3nh), (n,n′dt), (n,4n2p)
218	(n,3nα+)	(n,3nα), (n,4nh), (n,5n2p)
219	(n,pα+)	(n,pα), (n,dh), (n,n′ph)
220	(n,dα+)	(n,dα), (n,n′pα), (n,n′dh)
221	(n,tα+)	(n,tα), (n,n′dα), (n,n′th), (n,2npα)
222	(n,n′tα+)	(n,n′tα), (n,3npα)
223	(n,n′2α+)	(n,n′2α), (n,3n2pα)
224	(n,t2α+)	(n,t2α), (n,n′d2α)
225	(n,ph+)	(n,ph), (n,n′3p)

If data in the Cache from one of the source libraries are required in the EAF library, but the reaction is currently not in Master, then it is possible to add the reaction (which will both add the Reaction details in Parameter and copy the data to Master) by clicking the File|Add to Master menu item. If the reaction is already in Master, but the source of data needs to be changed then this can be done by clicking the File|Replace in Master menu item. A similar replacement can be made in the Final database by clicking the File|Replace in Final menu item. Prior to changes being made, confirmation dialogs similar to Figure 77 are displayed. If the selected reaction is from Master, then the File|Copy to Test menu item is enabled. If the reaction has preliminary modifications and/or modifications

then it is possible to carry out the modifications from the two viewing windows (Figure 106 and Figure 115) and put the data for the reaction into Test. If no modifications exist, then clicking this menu item will put a copy of the Master data into Test. Clicking the File|Create Test for all target's Final reactions menu item creates data in Test for all reactions in Final for the selected target.

If the data in the Cache are changed while the Cache contents window is open, then the reactions listed can be refreshed by clicking the View|Refresh data menu item.

Data can be placed in the Cache from other databases so that they can be visualised by clicking the File|Data selection… menu item or the first toolbar button. This displays the Data selection window shown in Figure 78. The available source databases are shown in the dropdown list, selecting one of these will show the targets present in the first list box, and selecting a target shows the reactions present in the second list box. Alternatively, one of the three SAFEPAQ-II databases can be selected from the list box. Whichever database is selected its path is shown at the top of the window. The data for the selected reaction are shown in the data grid. Note that if there are more than one final state then all the reactions are shown. The data grid shows the Multiplicity of the data, the *Q*-value (QI), the number of interpolation regions (NR) and number of data points (NP). Clicking the Copy to Cache button will add the data in the grid to Cache. Note that when Final data are transferred to the Cache a check is made to determine if the data are already in the Cache, if they are then these data are removed prior to copying.

If the selected database is Master, then an additional checkbox: Copy data as Test to Cache is available. Ticking this copies the data from Master to Cache and an additional copy is also copied to Cache as Test.

If the Copy all reactions for target check box is ticked, then clicking the Copy to Cache button copies all reactions for the selected target to the Cache. This is extremely useful if summed reactions with MT>200 are required. A time saving feature introduced from EASY-2005 means that when the Data selection window is opened the database and target that were selected when the window was last closed are again selected.

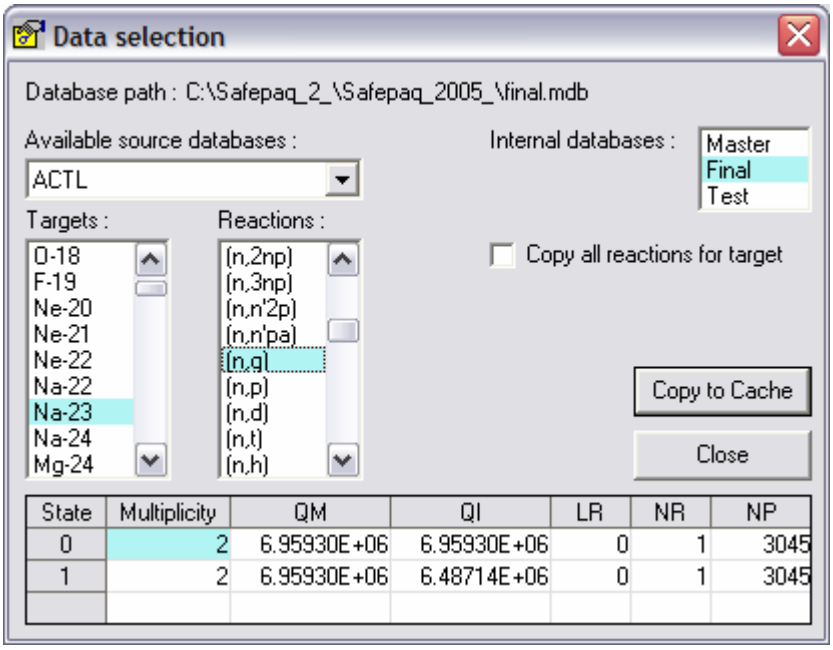


Figure 78. The Data selection window.

The lists of targets and reactions shown in the Targets and sources window (Figure 63) are shown by default and refer to 'normal' plots. If the Visualisation|Extended plots menu item in the main window (Figure 2) is checked then only those targets which have the full range of summed reactions with MT> 200 present are shown. Similarly the number of reactions is different and refer to the summed reactions such as (n,xp), (n,α+) and one termed 'Multiple'. The latter refers to the reactions (n,γ), (n,p), (n,d), (n,t), (n,h), (n,α), (n,2n), (n,3n) and (n,n′α). When the Plot button in Figure 63 is clicked then a series of cross section curves are plotted. Experimental data symbols are shown for each reaction type and if EXFOR data are overplotted then separate colours refer to data for the various reaction types.

If the Visualisation|Extended plots, use (n,n′p) not (n,g) menu item in the main window (Figure 2) is checked then in the multiple plot case data for the reaction (n,n′p) rather than (n,γ) are displayed. These extended plots are very useful for comparing several reaction types and investigating relationships between them. An example of such a plot, for (x,nx) reactions on ^{184}W is shown in Figure 79.

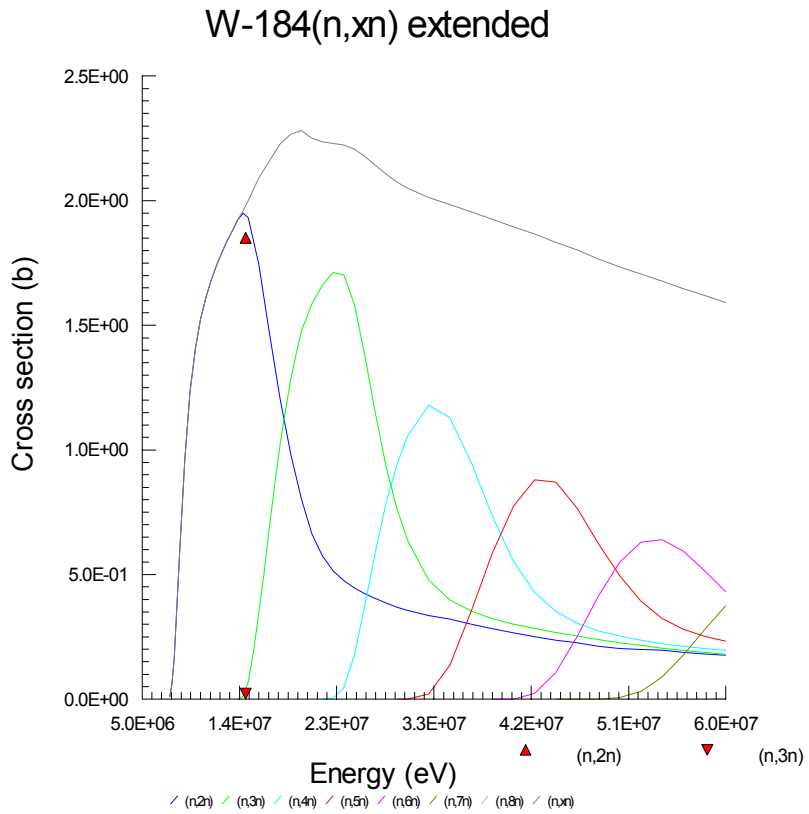


Figure 79. Plot of ^{184}W(n,xn) cross sections produced using the Extended plot option.

Integral data

Measurements can be made in a neutron spectrum, rather than at a particular neutron energy, to give an average cross section. In order to use such integral measurements to improve the data library it is necessary to be able to average the library data in well defined neutron spectra. Clicking the Integral data|Neutron spectra… menu item displays the Neutron spectra window shown in Figure 80.

Note that at the present time there are no integral data stored for deuteron- or proton-induced reactions. Consequently, there is no option to view spectra for these particles.

The available neutron spectra, which are stored in the Parameter database are displayed, followed by the type, a description and reference. A spectrum can be removed by clicking the Delete button. A further spectrum can be added by clicking the Add… button which displays the Add spectrum window shown in Figure 81. A name and description are entered in the text boxes, and a type (number of groups and weighting) is chosen from the dropdown list. The file

containing the spectrum is selected using the browse button (…) and the reference is selected from the dropdown list. Note that the file should be in standard 'ASCII' format ('%' character at the start of comment lines) with the `asc` extension. Clicking the Add button will add the spectrum to the database.

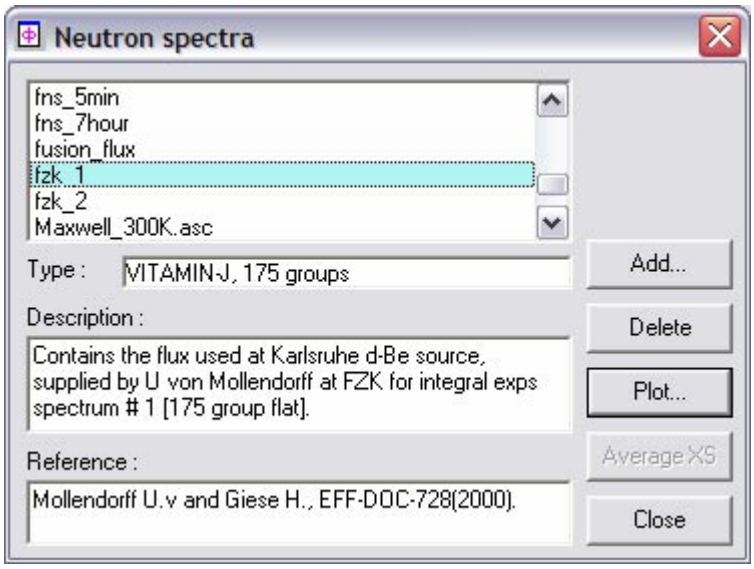


Figure 80. The Neutron spectra window.

A neutron spectrum can be plotted by selecting it in Figure 80 and then clicking the Plot… button. This displays the Plot spectrum window shown in Figure 82. This gives three options for plotting, showing the neutrons per energy group, per energy interval or per lethargy interval. The spectrum can be scaled by a factor entered in the text box, this is useful if it is required to compare two spectra with very different normalisations. Select one of the radio buttons and then click the Plot… button to display the Neutron spectrum window shown in Figure 83.

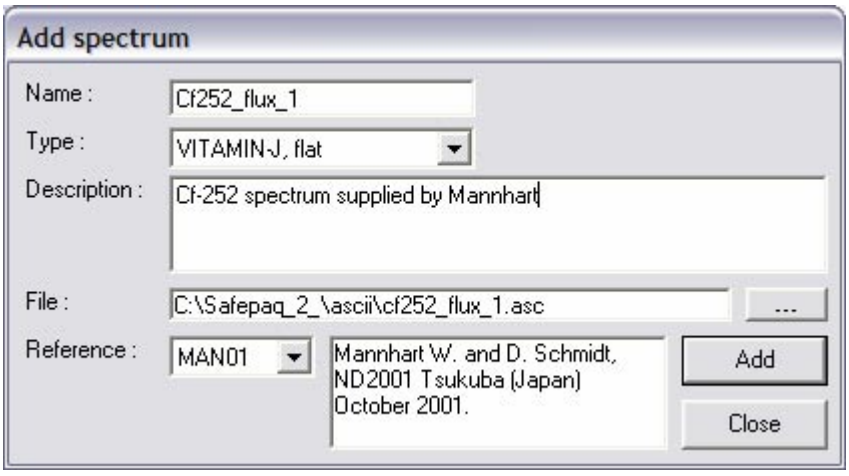


Figure 81. The Add spectrum window.

The menu bar in Figure 83 allows the plot to be printed to the default printer by clicking the File|Print menu item, and copied to the clipboard by clicking the Edit|Copy menu item. It is possible to compare two spectra by plotting them on the same graph. To do this a spectrum must be stored by clicking the Store|Store spectrum menu item (the name will then be shown in Figure 82 when this is subsequently opened again). The Neutron spectrum window is then closed and another spectrum chosed in Figure 80. Having plotting this, clicking the Store|Plot store menu item then displays both spectra.

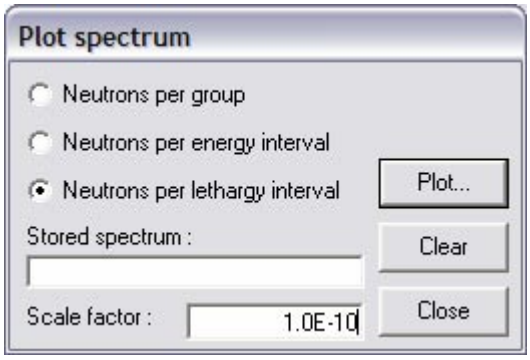


Figure 82. The Plot spectrum window.

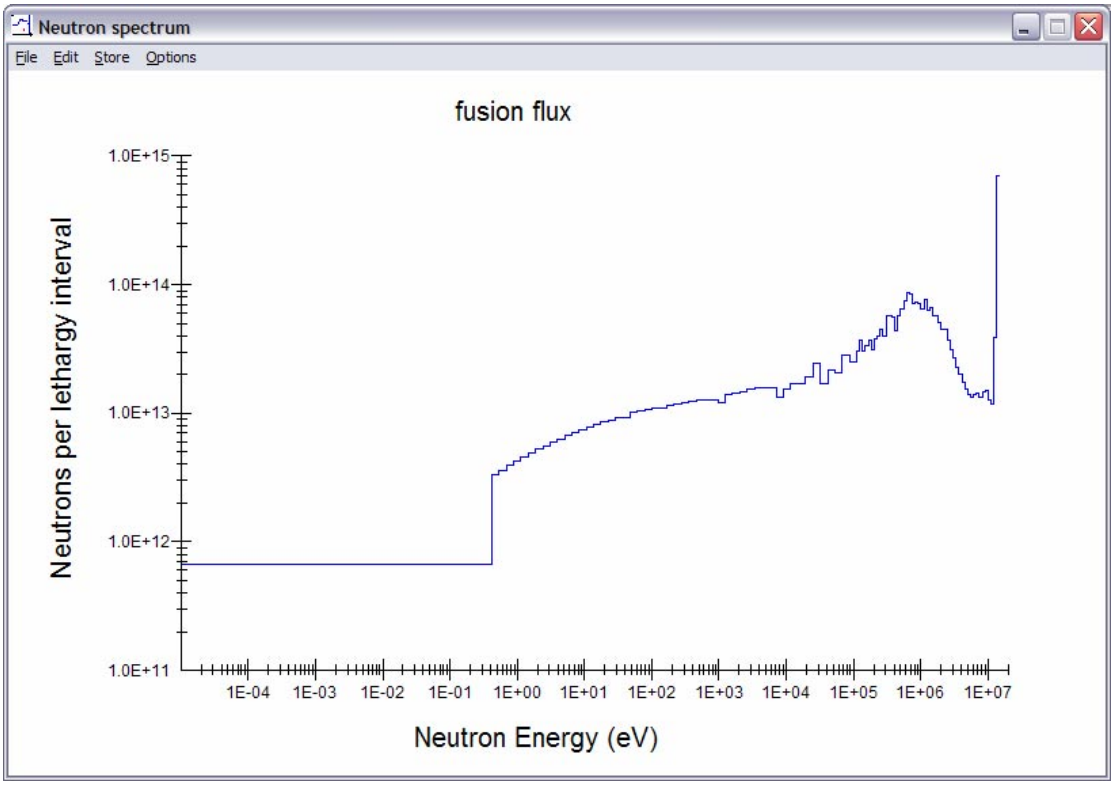


Figure 83. The Neutron spectrum window.

The y-axis can be plotted either linearly or logarithmically by clicking Options|y axis which displays a submenu with Log and Lin items. The axis ranges can be changed by clicking the Options|Axis scale… menu item which displays the Axis

scale window shown in Figure 84. Change the values in the text boxes and then click the Apply button to change the ranges. Clicking the Options|Thick lines menu item shows the lines as thick lines, which makes them more visible if the graph is copied and then pasted into another application.

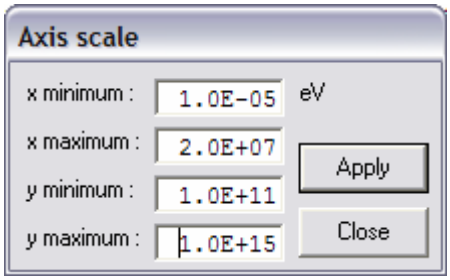


Figure 84. The Axis scale window.

Once the multi-group cross sections have been calculated, the Average XS button in Figure 80 becomes enabled. Clicking this once a spectrum is selected will calculate and store the average cross section for each reaction (this is the same as the 'collapsed' cross section calculated in FISPACT). These can then be compared with experimental integral data.

The values of the average cross sections for particular spectra can be seen by clicking on the Integral data|Average cross sections… menu item in the main window, which displays the Average cross sections window shown in Figure 85. Select a target, reaction and neutron spectrum in the three list boxes, click on the required radio button in the Final state group and then click the Get average to show the average cross section value in the text box.

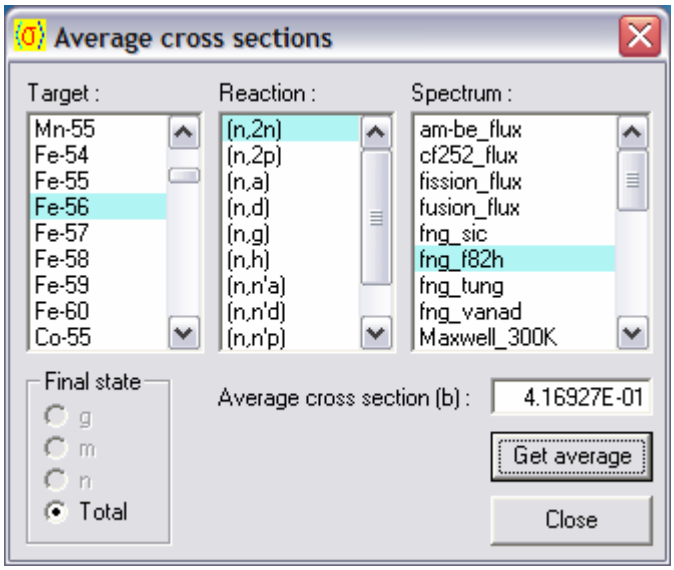


Figure 85. The Average cross sections window.

The experimental integral data can be viewed by clicking on the Integral data|View Integral data… menu item or the sixteenth toolbar button, which displays the Integral data window shown in Figure 86. Selecting a target shows which reactions have data, and selecting a reaction displays the available data in the grid. In addition to the spectrum name, cross section and uncertainty shown in the first three columns, the final column shows a flag. This indicates whether the data are to be used (so allowing several data in the same spectrum). The source of the data is indicated by a reference, where this is known.

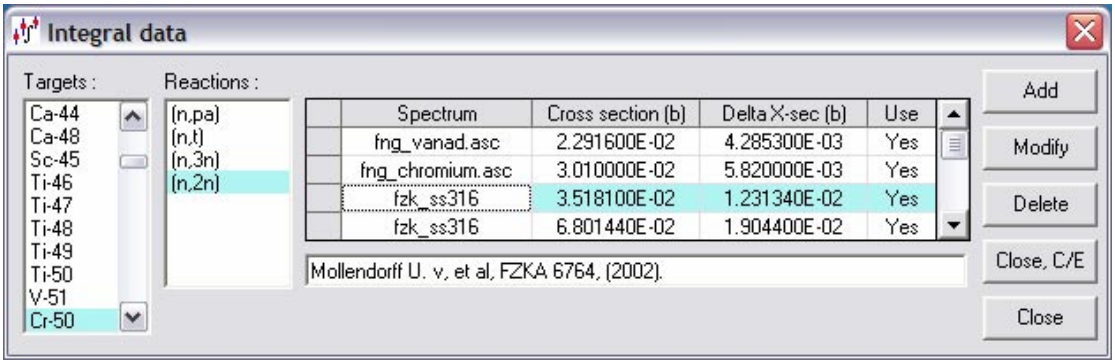


Figure 86. The Integral data window.

Clicking the Modify button will display the selected data in editing boxes below the reference. Changes to the data values or the flag can then be made and saved to the database by clicking the Save button. A data point can be removed by clicking the Delete button. A new data point can be added by clicking the Add button. This displays the dialog shown in Figure 30. Clicking the No button displays the Add Integral data window shown in Figure 87. Enter target and reaction details in the first text box, the dropdown list and with the Final state radio buttons. Enter the integral data in the text boxes and tick the Use check box. The default cross section unit is b, but by clicking the # button it is possible to toggle between b and mb for data entry. Note that the # button should be clicked prior to data entry. Select a reference from the dropdown list. Clicking the Add button will save the data in the Parameter database.

Note that the Save button actually becomes the Close, C/E button which acts as a shortcut to displaying the Integral C/E window when a change to the data is not in progress. Clicking this will close the Integral data window (as does the Close button) and open the Integral C/E window.

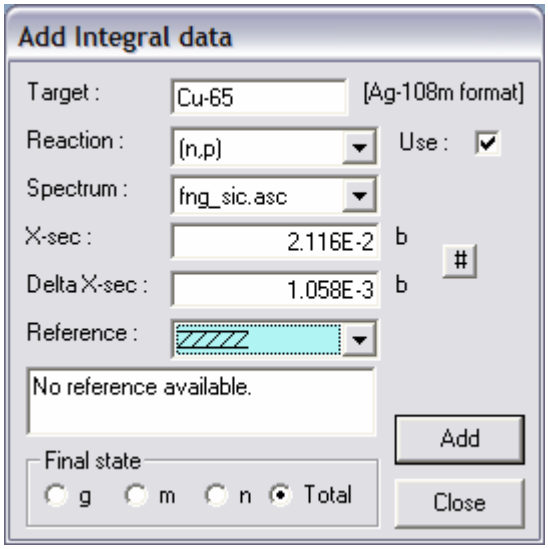


Figure 87. The Add Integral data window.

The reactions that can be selected in the Add Integral data window (Figure 87) include the various summed reactions with MT identifiers > 200 (see Table 1). In some cases experiments have been carried out on elements rather than isotopes. In order to improve the estimation of the isotopic effective cross section from the elemental value under the assumption that the elemental value applies to the most abundant isotope, a calculation can be carried out using the current cross section values.

Clicking the Integral data|Elemental analysis… menu item displays the Elemental analysis window shown in Figure 88. The element, spectrum and reaction are selected from the dropdown lists and the elemental cross section and uncertainty are entered in the text boxes. The required isotope (generally the most abundant) is selected by clicking one of the radio buttons to the left of the table and the Get data button is clicked. The particle production cross sections for the various isotopes are calculated and entered in the third column of the table. When all the cross sections have been calculated then the sum is formed and the k_i values defined in equation (2) are calculated and displayed in the fourth column. In equation (2) the cross sections (σ_i^c) are the library values, while f_i are the abundances. Finally the isotopic cross section value is displayed in the text box.

$$k_i = \sigma_i^c \Big/ \sum_j f_j \sigma_j^c \qquad (2)$$

By default the natural abundances are displayed in the second column. By clicking on the Enriched radio button it is possible to edit the abundance values to the required values. As can be seen from Figure 88, the isotopic value is generally similar to

the elemental value, but this depends on the actual cross sections for the selected element.

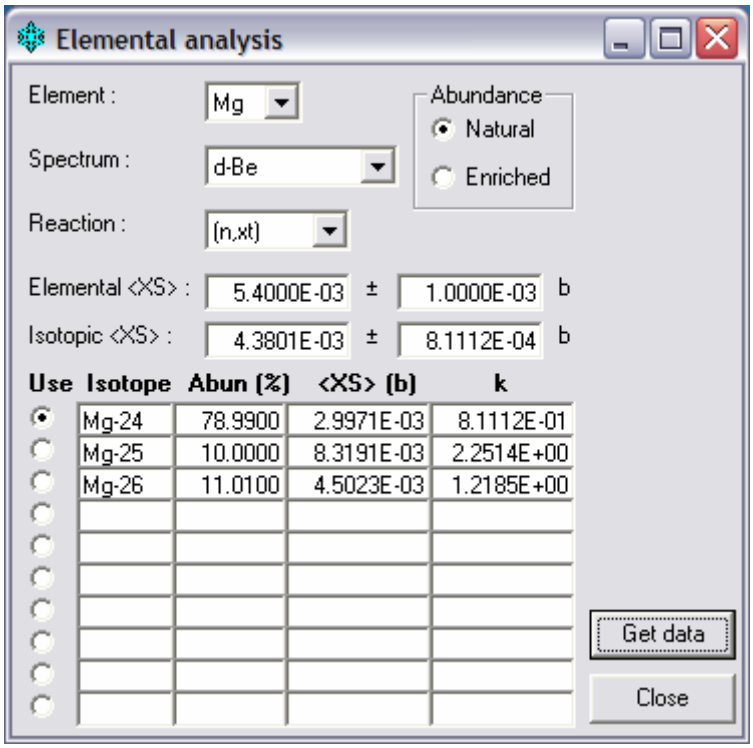


Figure 88. The Elemental analysis window.

Selecting a data set in Figure 86 stores details of the reaction and writes the reaction name in the main window status bar. Closing Figure 86 retains details of the selected reaction and enables the Integral data|Integral C/E… menu item. Clicking this displays the Integral C/E window shown in Figure 89 (the reaction is shown in the title bar). This initially shows the same integral data as in Figure 86 (but only where the Use flag is 'Yes') and if the multi-group cross sections have been calculated then the average cross section for the reaction using data in Final are presented with the C/E value. If the multi-group data have not yet been calculated then '????' is shown. Note that if a particle production cross section is selected then the calculation of the C/E values takes some time, and the user is warned by a message in the Staus bar to have patience. If the data are in Final then the Plot… button is enabled – its use is described below. If the reaction is in Test then the Test button is enabled. Selecting one of the spectra enables the Reaction rate… button. Clicking the Copy button places the entire contents of the data grid on the clipboard.

Clicking the Test button will expand the window, change the heading of the third column from 'Final' to 'Test', change the values displayed in the grid and display another grid. This enlarged window is shown in Figure 90, showing the multi-

group data calculated using Test and several new buttons and controls.

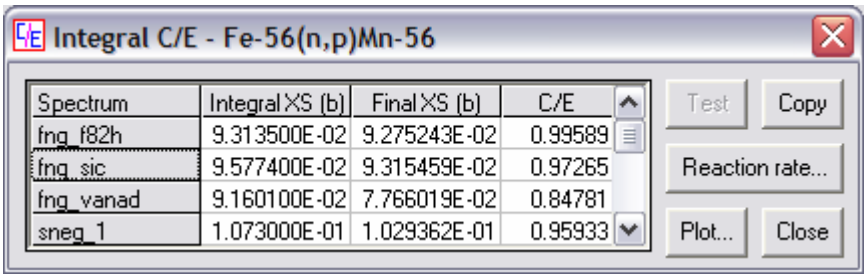


Figure 89. The Integral C/E window.

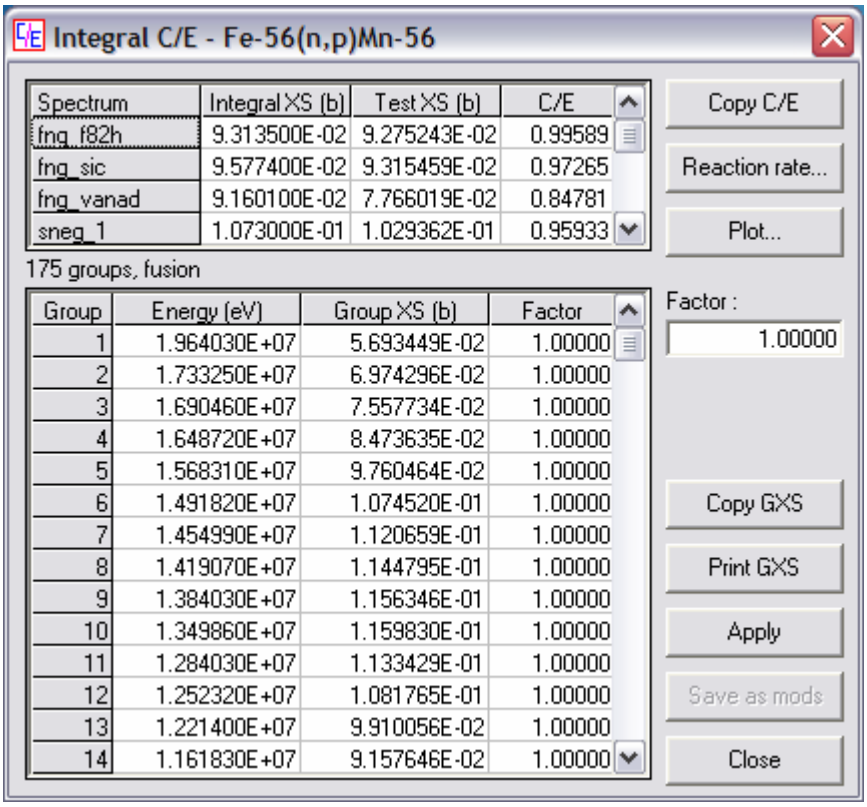


Figure 90. The C/E Integral data window (enlarged).

Clicking on a spectrum displays the group cross sections in the lower grid, the number of energy points and the weighting are shown above the lower grid. Initially the Factor for each group value is 1.0. If it is required to alter the group data to get a better C/E value, then select the required groups and alter the factor in the text box. Clicking the Apply button will display the new factor in the lower grid, recalculate the C/E value and display it in the upper grid and enable the Save as mods button. Note that all spectra with the same number of groups (irrespective of the weighting) have their C/E values updated. Clicking the Save as mods button will find a set of modifications (Mod type 4) for the correct energy ranges and store them in Parameter. It will also remove from the Test

database the current reaction. This forces the reaction to be remade using the modifications before it can be used again.

Clicking the Copy GXS button copies the selected data in the lower grid to the clipboard. Clicking the Print GXS button prints the entire contents of the lower grid to the default printer. Clicking the Copy C/E button copies the entire contents of the upper grid to the clipboard.

In both Figure 89 and Figure 90 there is a Reaction rate… button. If the one in Figure 89 is clicked then the reaction rate data for the reaction in Final are plotted. If the one in Figure 90 is clicked then the data in Test are plotted. The graphs are displayed in the Reaction rate window shown in Figure 91. What is plotted is shown in equation (3), where the reaction rate in the *i*th group is shown in terms of the group cross sections (σ_i) and group fluxes (ϕ_i). It gives a visual indication of the energies at which the cross section in a particular spectrum contribute significantly to the production of the daughter nuclide. This can be used to indicate where changes in the cross section should be made so as to improve the C/E value.

$$R_i = \sigma_i \phi_i \Big/ \sum_j \phi_j \qquad (3)$$

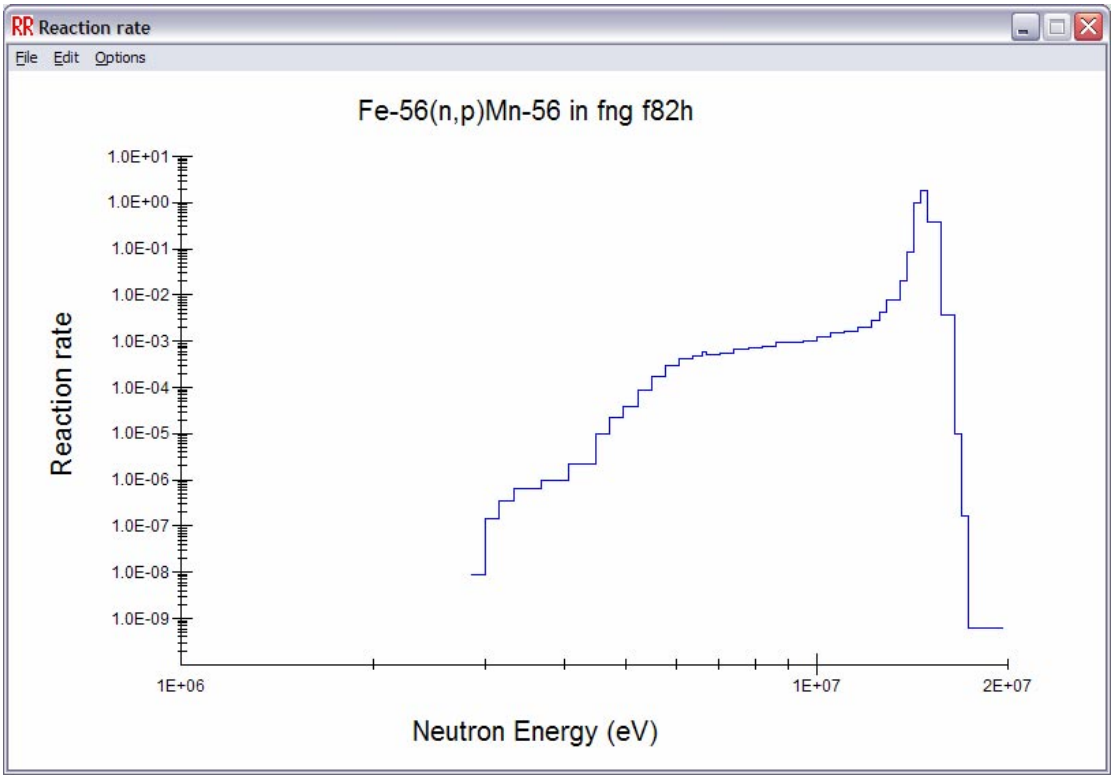


Figure 91. The Reaction rate window.

The menu bar in Figure 91 allows the plot to be printed to the default printer by clicking the File|Print menu item, and copied

to the clipboard by clicking the Edit|Copy menu item. The y-axis can be plotted either linearly or logarithmically by clicking Options|y axis which displays a submenu with Log and Lin items. The axes ranges can be changed by clicking the Options|Axis scale… menu item which displays the Axis scale window shown in Figure 84. Change the values in the text boxes and then click the Apply button to alter the ranges.

Returning to Figure 90, clicking the Plot… button displays the Integral C/E graph window shown in Figure 92. This shows the C/E values for the various neutron spectra with error bars representing the experimental uncertainty. If uncertainty data exist in the Final database then the uncertainty value for the reaction is used to display an error band around the C/E = 1 value. If the Options|Show values menu item is checked then the C/E values are displayed next to each point and on the error band. The graph can be printed to the default printer by clicking the File|Print menu item, and copied to the clipboard by clicking the Edit|Copy menu item.

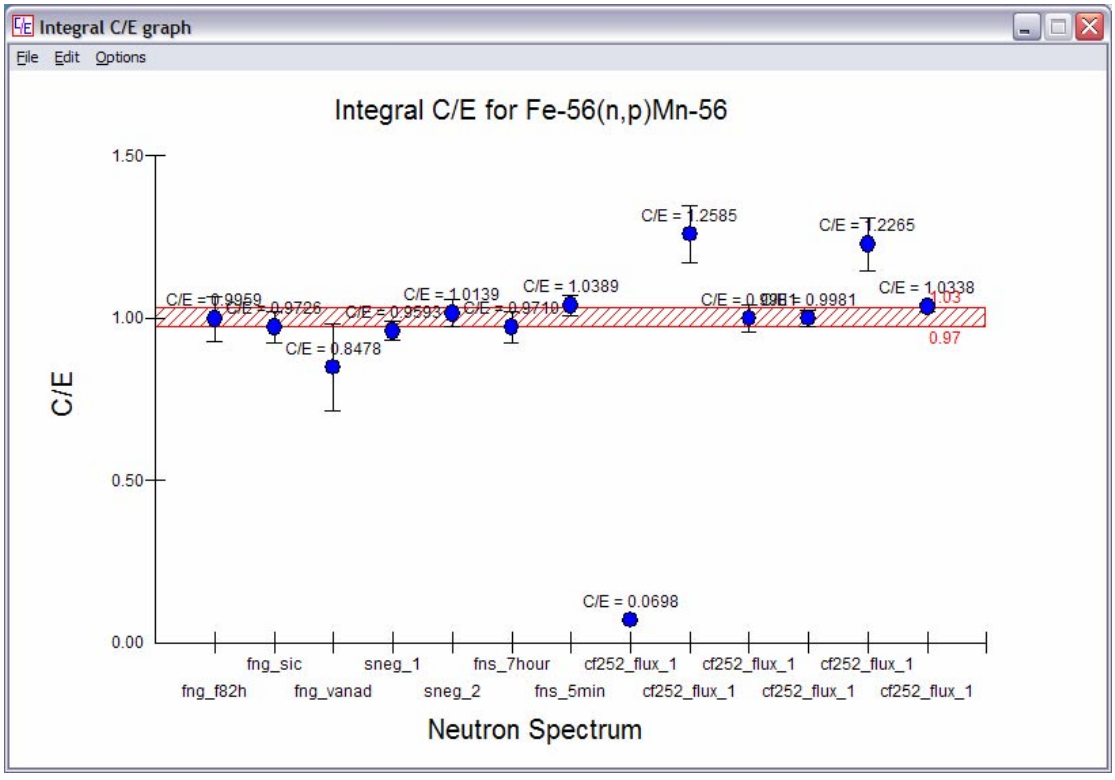


Figure 92. The Integral C/E graph window.

Since EAF-2007 it is possible to display the C/E values in another way. Selecting the Integral data|Extended C/E plot menu item in the main window checks it and means that when the Plot… button in Figure 89 is clicked then the Integral C/E graph (Extended) window shown in Figure 93 is displayed. In this case the reaction rate for each spectrum is calculated and

the point is placed at the energy corresponding to the maximum reaction rate. The energy interval such that 90% of the reaction rate is contained is calculated and used to plot an energy 'error bar'. Such a plot shows clearly the energies at which the integral data can be used to validate the EAF data.

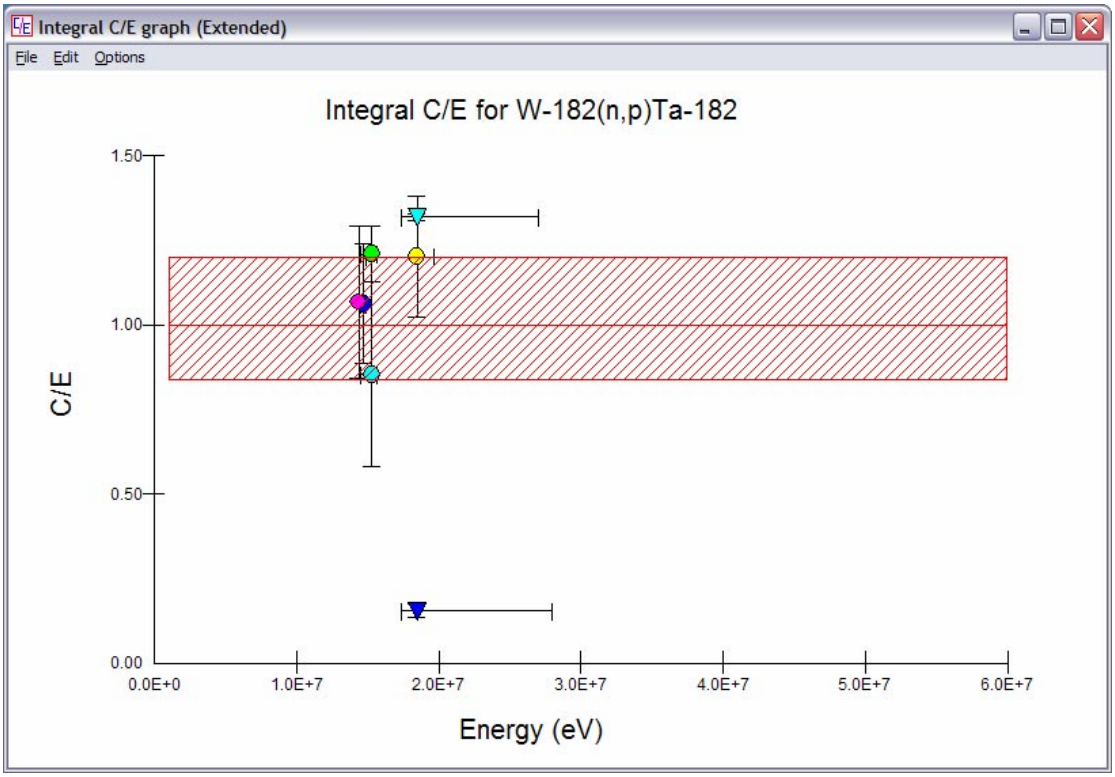


Figure 93. The Integral C/E graph (Extended) window.

The File|Print, Edit|Copy and Options|Axis scale… menu items are the same as in the Integral C/E graph window (Figure 92).

If the Options|x axis ticks menu item is clicked then a sub-menu opens with the menu items 1 – 6 shown. Checking one of these displays the graph with the corresponding number of x axis tick marks. In Figure 93 six tick marks are shown. If the Options|y axis ticks menu item is clicked then a submenu opens with the menu items 1 – 5 shown. Checking one of these displays the graph with the corresponding number of y axis tick marks. In Figure 93 three tick marks are shown.

If the Options|Show values menu item is clicked then a submenu opens with the menu items None, All, Band and Points shown. Checking All displays the mean energy and C/E values next to each point and the library uncertainty next to the error band. Band only displays the library uncertainty next to the error band, Points only displays the mean energy and C/E values next to each point. None removes all values.

If the Options|Legend menu item is clicked then a submenu opens with the menu items None, Right, and Bottom shown. Checking Right displays the spectrum name for each point in a legend at the right of the graph. Checking Bottom displays the spectrum name for each point in a legend at the bottom of the graph. None removes the legend.

The above discussion refers to comparing the data in Final (or Test) with the experimental integral data. It is also possible to do the same comparison using data from one of the data sources. The choice of source library is made by clicking on the Integral data|Select Source library… menu item which displays the Select Source library window shown in Figure 94. Select the required source and then click the Select button.

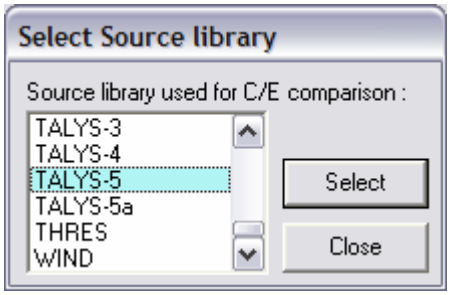


Figure 94. The Select Source library window.

The Integral data|Integral C/E for <Source>… menu item in the main window is enabled, for example if the TALYS-5 source is selected then it reads Integral C/E for TALYS-5…. Clicking this displays the Integral C/E for TALYS-5 window which is identical to Figure 89 (except that the name of the data source is shown in the title bar). The data for the selected reaction in the source are collased with the required neutron spectra. Only data for the selected reaction are processed in this way, the progress of the generation of the multi-group data for the various group structures can be seen in the main window status bar. The plotting of graphs for the selected source follows exactly the description given above for data from Final.

Reaction data

The next objective of SAFEPAQ-II is the processing of reaction data to produce EAF data files. Based on the ideas used in SYMPAL this consists of a number of well defined steps.

- Construct a list of reactions that are required in the library.
- Decide on the source of data for each reaction.
- Compile data from these sources into the Master database.
- Based on the experimental data and systematics held in the Parameter database, construct a set of modifications, which

when applied to the data in Master produce the data in the Final database.

- Use Final to produce a summary of each reaction (thermal, 30 keV, 14.5 MeV and 20 MeV cross sections and the resonance integral).
- Produce the multi-group data (stored in Final).
- Produce the uncertainty data (stored in Final).
- Carry out internal validation against the data held in Parameter (Validation plots).
- Write out the point wise, group wise and uncertainty files in EAF format.
- Produce the various items of documentation (REPORT file and reaction list).

Each of these steps is accomplished by using items on the Reaction data menu, they are all described below.

Clicking the Reaction data|Reaction list menu item or the twenty-second toolbar button displays the Reaction list window shown in Figure 95. Enter an element symbol in the first text box and click the Get data button to show the nuclides for the entered element in the Targets list box. Select a target and all the reactions along with the existing source of data are shown in the large list box. If the Select previous reaction option is checked and a reaction is selected, then when another Target is selected the reaction type (now shown in the Select previous reaction text) is automatically selected. A ToolTip shows the reaction number and the multiplicity of the selected reaction. The source of data for a particular reaction can be changed by clicking the Modify… button. This displays the Modify reaction window shown in Figure 96.

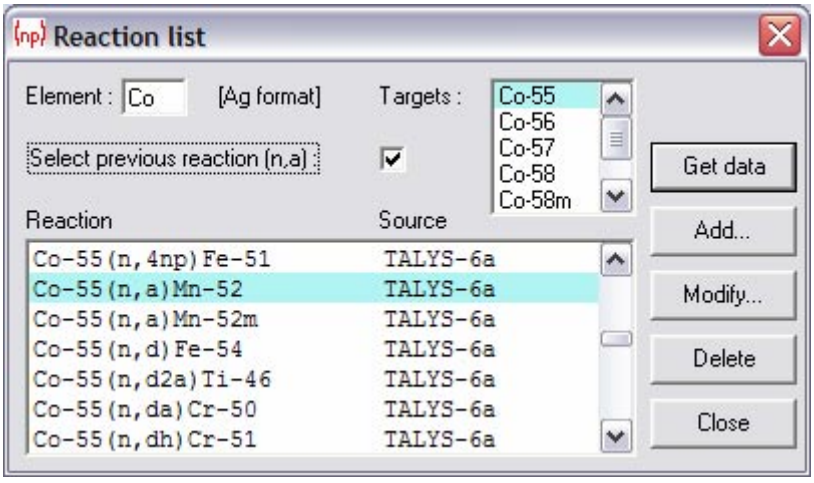


Figure 95. The Reaction list window.

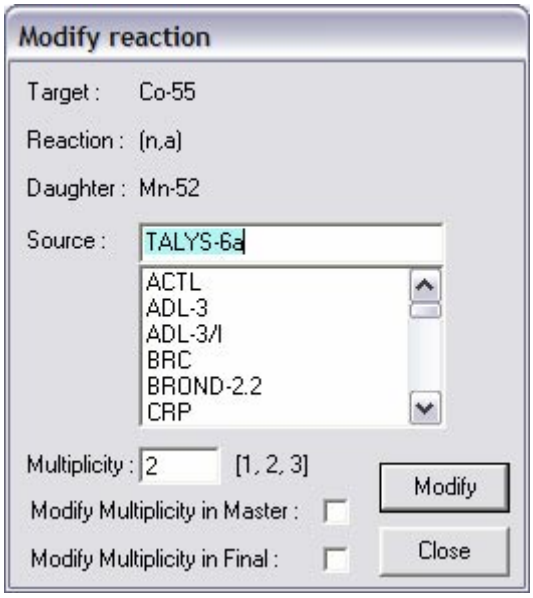


Figure 96. The Modify reaction window.

The current source of the selected reaction is displayed, and the available data sources are shown in the list box. The current multiplicity of the reaction (number of final states) is shown in the Multiplicity text box. A new source and/or multiplicity can be selected from the list box and entered in the text box. Clicking the Modify button will save the data in the Parameter database. Note that if the multiplicity of a reaction is modified using this window after the Master and Final databases have been generated then it is necessary to also modify it in them. Depending on the stage of processing that has been reached, then the Modify Multiplicity in Master and/or Modify Multiplicity in Final options should be checked prior to clicking the Modify button.

Clicking the Add... button in Figure 95 displays the Add reaction window shown in Figure 97.

The target of the new reaction is entered in the first text box (by default the target in the Reaction list window (Figure 95) is entered), the reaction is selected from the dropdown list, the data source is selected from the list box and the multiplicity and final state are entered in the text box and selected with the radio buttons. Clicking the Add button will save the data in the Parameter database. Note that if the reaction list is being added to after the Master and Final databases have been generated then it is necessary to add data for the new reaction to them. Depending on the stage of processing that has been reached, the two Add data to <Name> databases check boxes should be ticked or cleared.

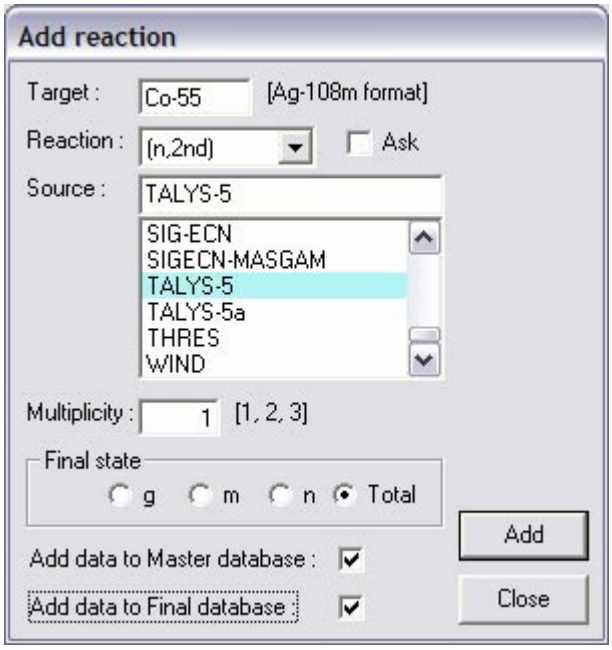


Figure 97. The Add reaction window.

If the reaction does not exist in the selected data source then the most sensible alternative will be used, if possible, by default. Thus if the reaction is (n,d) and only (n,n′p+d) data exists in the source then data for this reaction will be used. If the Ask check box is checked then a dialog will confirm this.

Clicking the Delete button in Figure 95 removes the reaction from the *ReacSummary* table in the Parameter database.

The tasks of adding and deleting reactions and changing the data source for an existing reaction are common during library preparation. There are several ways of achieving these tasks in SAFEPAQ-II and the following recommendations are made for carrying them out efficiently. Prior to the generation of Master and Final is the best time to add or delete reactions and the Reaction list window (Figure 95) is the best place to do this. The data source can also be changed using the Modify reaction window (Figure 96) at this stage, but if Master and Final have already been produced then the Single reaction window (Figure 119) is to be preferred. Note that if the Modify reaction window (Figure 96) is used to change the source and Master already exists then this will cause problems as the Reaction list window (Figure 95) will show this change (reflecting the change in Parameter), but Master will still contain the original source.

It is possible to change all instances of a data source to another for all targets in a specified ZAI range (ZAI = 10000 x Z+10 x A + I). Clicking on the Reaction data|Global source replace… menu item displays the Global source replace

window shown in Figure 98. Enter the original and new data source identifiers and the ZAI limits in the text boxes and click the Replace button to make the change.

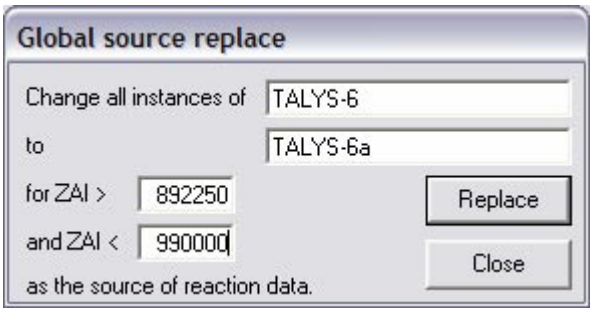


Figure 98. The Global source window.

When moving from an EAF library with an upper energy limit of 20 MeV to one with 60 MeV, a considerable number of reactions need to be added. In the construction of EAF-2005 the TALYS data source was used extensively. Reactions present in TALYS but not in the previous EAF library (EAF-2003) needed to be added. This can be done by clicking on the Reaction data|Add new reactions… menu item that displays the Add new reactions window shown in Figure 99. A choice of which reactions to include is made by entering a value in the text box. If the reaction in TALYS has a maximum cross section at some energy greater than this value then the reaction is added to the *ReacSummary* table in Parameter. Clicking the Add button adds all the relevant reactions.

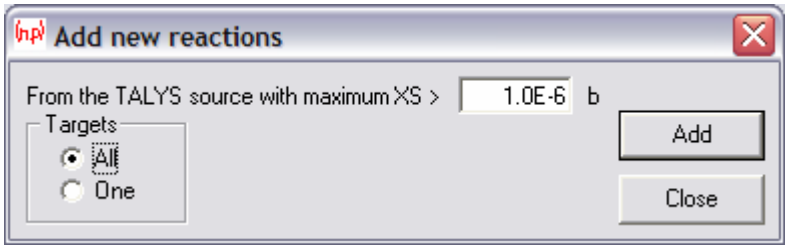


Figure 99. The Add new reactions window (All option).

This is the default behaviour, with the All Targets option selected. If the One Targets option is selected then the window will be displayed as shown in Figure 100. This enables reactions for only the specified target with large enough cross section to be added from TALYS.

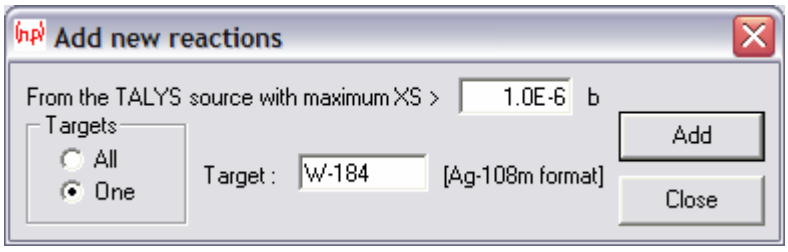


Figure 100. The Add new reactions window (One option).

In the Add new reactions window (Figure 99) and several other windows the word TALYS appears. There are several data sources of this type and the one that is required to be used is entered in the Version of TALYS text box in the Settings window (Figure 1).

During the development of deuteron and proton libraries it is common to start with a reaction list for neutron-induced reactions. When the incoming particle in the list is changed form n to say d, then many of the reactions in the list will be elastic reactions such as (d,d) where the daughter is not an isomeric state. These reactions can be removed from the list by clicking the Reaction data|Delete elastic reactions menu item.

Reading the Log and checking on errors often requires that the reaction number in the Final database be identified. This is possible by clicking on the Reaction data|Reaction numbers menu item that displays the Reaction numbers window shown in Figure 101. Enter the reaction number in the text box, click the Get details button and the reaction and source are shown.

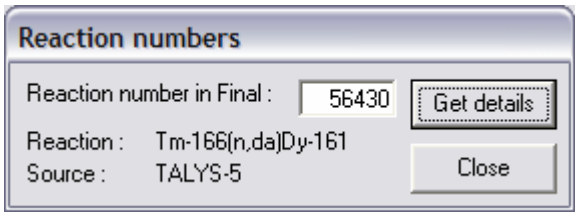


Figure 101. The Reaction numbers window.

Clicking the Reaction data|Reaction search menu item or the twenty-third toolbar button displays the Reaction search window shown in Figure 102. Using this window searches can be made for particular reaction types or data sources. If searching by reaction type then select the Reaction radio button and select a reaction type from the dropdown list and choose the initial and final states with the radio buttons. Clicking the Get reactions button shows all reactions that fit the criteria, the data source and the total number of reactions. This list can be printed out by clicking the Print button and placed on the clipboard by clicking the Copy button.

If the Score check box is checked then the search can be refined by specifying a score; then only reactions with that score are returned. If the Show systematic UseR check box is ticked then the status of this flag is also returned. '+' indicates the flag is set, '-' that it is cleared and ' ' indicates that the reaction has no systematics flag. If searching by reaction type then there is an additional option to sort the reactions by target (the default) or by data source (then within that source by

target). To do this click the right hand radio button above the list box.

If a search by data source is required then click the Source radio button and select the source from the dropdown list. Clicking the Get reactions button shows all reactions that fit the criteria, the data source and the total number of reactions.

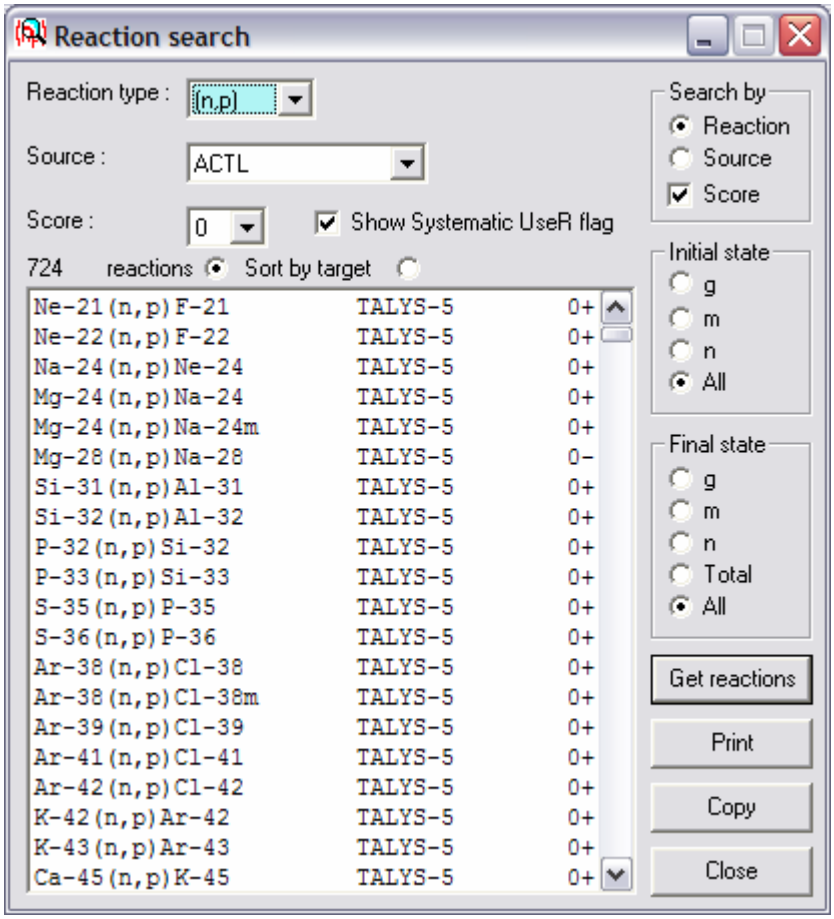


Figure 102. The Reaction search window.

Another way of making global changes of the data source for sets of reactions is by considering the Quality score for the reaction (see Table 3). By clicking on the Reaction data|Change data source for score=0 to TALYS for reaction type menu item and then selecting a reaction type such as (n,2n) from the submenu, then all (n,2n) reactions that have score = 0 and with a data source not set to TALYS will be changed to data from the current TALYS version. The submenu shows fifteen reaction types explicitly. All the remaining reaction types can be changed together by clicking the Others menu item.

After making significant changes to the reaction list it is sensible to check that all the specified data sources for each reaction actually contain data. This can be done by clicking the Reaction data|Check|Sources in reaction list… menu item

which displays the Check sources in reaction list window shown in Figure 103.

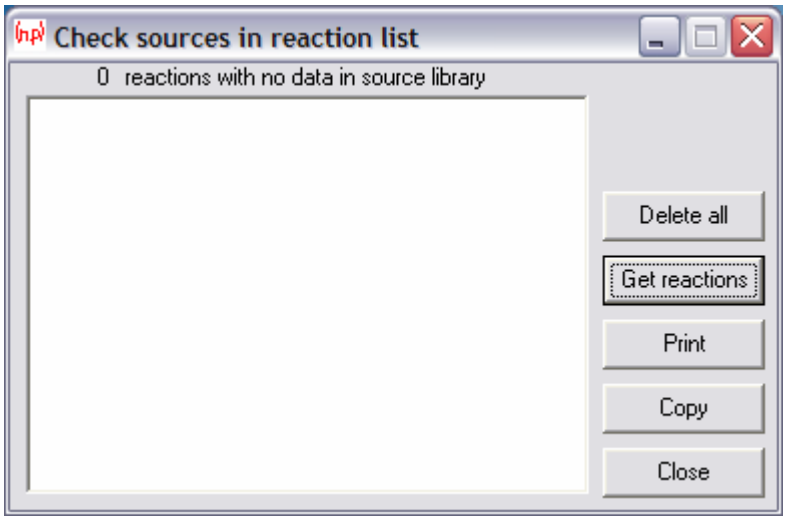


Figure 103. The Check sources in reaction list window.

Click the Get reactions button to display a list of reactions for which the specified data source actually contains no data. The list can be printed out by clicking the Print button and placed on the clipboard by clicking the Copy button. During the production of the EAF-2007 proton-induced library there was only a single data source. Therefore all reactions listed needed to be removed from the reaction list. In such a case all the listed reactions can be removed by clicking on the Delete all button.

A second check that can be carried out is to check that all the reactions have daughters that are also defined in the list of nuclides. Problems may occur with reactions having isomeric daughter states not defined in the nuclide list. Clicking the Reaction data|Check|Daughters in reaction list… menu item displays the Check daughters in reaction list window which is identical to Figure 103, except that the text reads 'reactions with no decay data for daughters'.

A third check that can be carried out is to check that all the multiplicities are correct. Clicking the Reaction data|Check| Multiplicities in reaction list… menu item displays the Check multiplicities in reaction list window shown in Figure 104. Select one of the radio buttons specifying the multiplicity to test and then click the Get reactions button to display a list of reactions for which the multiplicity is incorrect. The list can be printed out by clicking the Print button and placed on the clipboard by clicking the Copy button

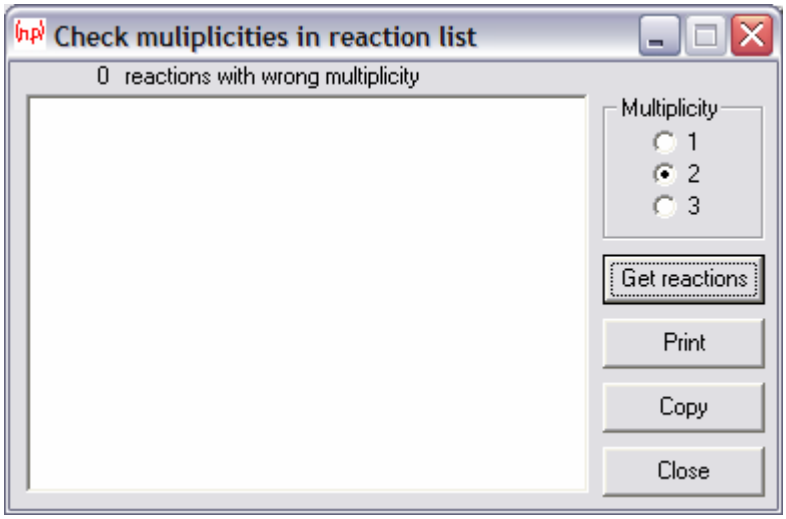


Figure 104. The Check multiplicities in reaction list window.

Having decided on the reactions and their sources the next step is to construct the Master database. This is done by clicking on the Reaction data|Generate Master database menu item. If Master already contains data then the confirmation dialog shown in Figure 105 is displayed prior to deleting any data. It takes a significant time (~ 7 hours) to generate Master.

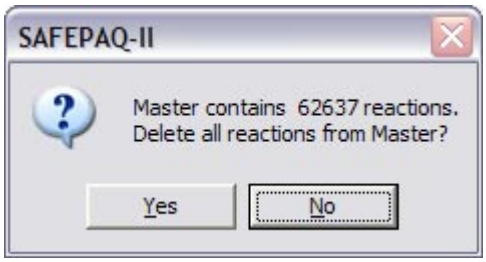


Figure 105. Confirmation dialog prior to deleting reactions from Master.

The next step is to find modifications to the data in Master. This is divided into two stages; termed preliminary modifications and modifications. In the first stage three types of preliminary modifications are considered. Firstly any pre-equilibrium modifications to capture data at high energies are found. SAFEPAQ-II carries out this step by comparing the Master data with that predicted by systematics at 14.5 MeV. Only reactions with a multiplicity of one are considered (to avoid issues with branching). Any reactions where (data in Master / Systematics) < 0.5 are noted and the additional data are generated using the Zhixiang and Delin formula for direct capture. This generates 119 (39 in the case of a non-extended energy library) data points in the energy range 1 – 60 (20) MeV, these are stored in the *Additional data* table of Parameter and a modification of Mod type 9 is stored for the reaction. Click on

the Reaction data|Find all pre-equilib preliminary modifications menu item to carry this out.

The data files contain 'double points'. These are where two data points have the same energy but different cross sections. Double points (and single points exactly at the E_H value for (n,γ) reactions) can cause problems. It is necessary to slightly shift the energy value of such points, clicking the Reaction data|Find all EH preliminary modifications menu item carries out this step.

Thirdly, it is possible that some data files contain inaccurate *Q*-values for the non-threshold reactions. These can be corrected by using data from the Wapstra mass table. Any reactions where the *Q*-value in Master differs by more than 5% from the Wapstra value are changed to the Wapstra value. Click on the Reaction data|Find all non-threshold Q-value preliminary modifications menu item to carry this out.

These three types of preliminary modifications involve several of the basic modifications considered in SAFEPAQ-II. The nineteen modification types are shown in Table 2. The results of these steps can be viewed by clicking the Reaction data|View preliminary modifications… menu item or the twenty-fourth toolbar button which displays the Preliminary modifications window shown in Figure 106.

Modifications are either introduced automatically during processing or in an 'Ad-hoc' fashion. For those added by processing there is a yellow background text box containing 'Process'. For Ad-hoc mods the box contains 'Ad-hoc' on a blue background. If the Change value of Kind check box is ticked in the Settings window (Figure 1), then it is possible to toggle the type by double clicking the coloured box with the mouse. This should not normally be necessary and the check box should normally be cleared. If the Ext check box is ticked then values of parameters for pre-modifications in the External database (see page 137) will be displayed in a ToolTip. If there is more than one pre-modification, then pressing the '>' or '<' keys will display the next or previous details. For some reactions there may be two data merge (Mod type 13) pre-modifications present. The order of these is important and it may be necessary to reverse them, which can be done by selecting the first data merge and then clicking the Switch button.

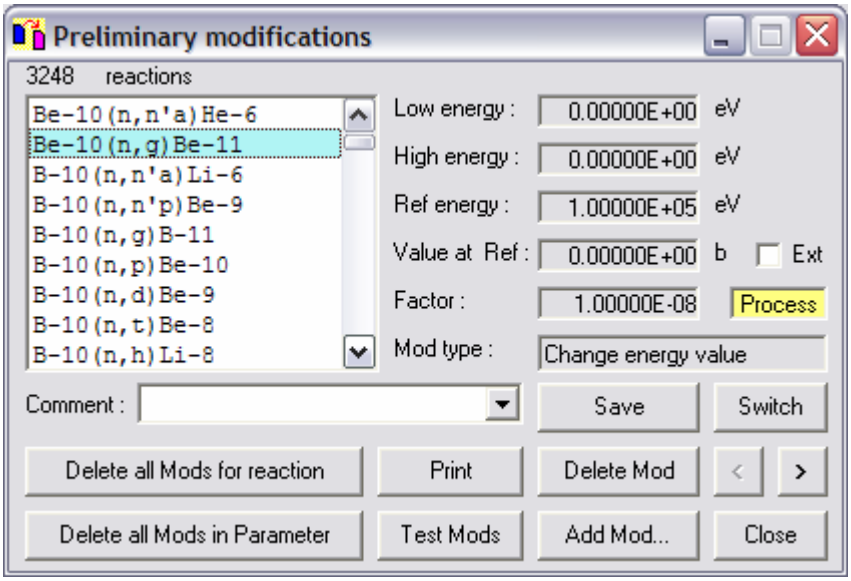


Figure 106. The Preliminary modifications window.

In Table 2 a brief description of the Action of each Mod type is given, followed by a specification in terms of the six fields used in each modification. These are [Elow], [Ehigh], [Eref], [Xref], [fact], [Addnum]. The first five are Double data types and the last is a Long. The first three are typically energy values, the fourth is a cross section, the fifth a factor and the sixth the identification number of additional data.

In Figure 106 values for the first five of these fields are shown in the text boxes and the Action of the modification is shown in the Mod type text box. The value of the Addnum field is rarely required, but it is available in a ToolTip by hovering the cursor over the Mod type text box. If a Mod Type 13 (data merge) modification is selected then the ToolTip also shows the upper energy (Emax) of the data merge. Selecting any of the reactions in the list box shows the values of the first five fields for the first modification in the text boxes. If there is more than one modification for the reaction then the > and < buttons are enabled, it is possible to view each of the modifications by clicking < to move back and > to move to the next one. The selected modification can be removed by clicking the Delete Mod button. Clicking the button actually inserts a Mod type 17 modification for the reaction. The reason is that this Ad-hoc deletion is stored and can be redone automatically for a future library. There may be times when the pre-modification needs to be removed completely and this can be done by clicking the Delete Mod button with the `Shift` key pressed. A new modification can be added by clicking the Add Mod… button which displays the Add Preliminary modification window shown in Figure 107. Note that if the `Shift` key is pressed while clicking the Add Mod… button, then the details of the currently selected reaction are added to Figure 107.

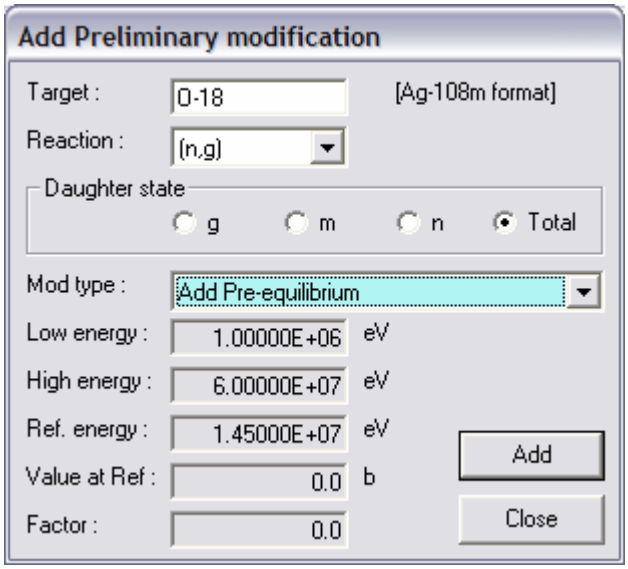


Figure 107. The Add Preliminary modification window.

Enter details of the reaction in the text box, dropdown list and with the radio buttons. Select a type of modification in the Mod type dropdown list and add any values required in the text boxes. Note that the boxes that require data are shown in white rather than grey. If the Data merge (Mod type 13) modification is chosen from the dropdown list then a list box of the source databases becomes visible. If the Low energy merge (Mod type 18) modification is chosen from the dropdown list then list boxes showing the source databases and the reaction types become visible. For both modification types it is necessary to select a database from the Source databases dropdown box which will provide the data for the reaction. In the Low energy merge it is possible to use data for a different type of reaction than the reaction specified in the Reaction dropdown box. To do this select a reaction for the low energy data from the Source dropdown box. Clicking the Add button will add the modification to the Parameter database.

Note that from EASY-2005 it is possible to do a data merge using data from a summed reaction rather than only for a reaction of the exact reaction type.

Table 2. Details of the modification types.

Mod type	Action	Specification
1	Extrapolated data points	Additional data points between [Elow] and [Ehigh] extrapolated using the law in [Xref].
2	Renormalise to systematics	Renormalise all data between [Elow] and [Ehigh] to the systematic value [Xref] given at 14.5 MeV or 30 keV [Eref].
3	Renormalise to experiment	Renormalise all data between [Elow] and [Ehigh] to the experimental value [Xref] given at [Eref].
4	Renormalise by factor	Multiplies all data between [Elow] and [Ehigh] by a factor [fact].
5	Removes data points	Removes all data points with [Elow] ≤ Energy ≤ [Ehigh]. Note that mod implemented for no points > [Ehigh] at this stage.
6	Renormalise by linearly energy dependent branching ratio	Multiplies each data point between E_H [Elow] and 60 MeV [Ehigh] by factor f. $f=f_{mid}+(f_{high}-f_{mid})*(E-E_{mid})/(E_{high}-E_{mid})$. E_{high}=[Eref], f_{mid}=[Xref], f_{high}=[fact].
7	Modification of *Q*-value	Replaces QI in the Reaction entry by the new *Q*-value [Eref].
8	Change number of points	Removes npt [Addnum] points from the start of cross section, replaces by 1 point [Xref] at E [Eref]. Adjusts NP in Reaction and Interpolation tables.
9	Pre-equilibrium addition	Additional cross section data between [Elow] and [Ehigh] given in [Addnum].
10	Change interpolation law	The interpolation law for points between [Elow] and [Ehigh] is changed to Int([fact]). ***Note*** that when entering [Elow] use a value ≥ than the value required.
11	1/v addition	Additional cross section data between 1x 10^{-5} eV [Elow] and E_V [Ehigh] given in [Addnum]. Curve can go through [Xref] at [Eref] if required.
12	Add a data scrap	Additional data between [Elow] and [Ehigh] given in [Addnum]. The interpolation law is Int([fact]) and the number of points is in [Eref].
13	Data merge	Additional data above [Eref] given in [Addnum]. The interpolation law is Int([fact]) and the number of point is in [Xref].
14	Change energy value	Data points at [Eref] are changed by a factor 1 ± [fact]. Lower point by (1-[fact]), the higher (if present) by (1+[fact]).
15	Change cross section	The data point at [Eref] has its cross section value changed to [Xref].
16	Add single data point	A new data point of cross section value [Xref]at [Eref] is added.
17	Delete modification	An existing modification of type [Addnum] with parameters given by [Elow], [Ehigh], [Eref], [Xref], [fact] is not used.
18	Low energy merge	Additional data below [Eref] given in [Addnum]. The interpolation law is Int([fact]) and the number of point is in [Xref].
19	Energy scale shift	All data points have energy value increased by [Eref].

In Figure 106, clicking the Delete all Mods for reaction button removes all preliminary modifications for the reaction from the database. Note that this method of deleting actually removes the modification rather than by inserting a Mod type 17 modification. It is possible to remove all preliminary modifications by clicking the Delete all Mods in Parameter button. It is possible to see the effect of modifications on a reaction by clicking the Test Mods button. This copies data from the Master to Test database, and carries out the

modifications. The cross section can then be visualised in the normal way by copying the data to Cache. It is possible to add a comment so that details of the added modification can be noted. To do this select the pre-modification and either type a comment or select an existing one using the dropdown list. Clicking the Save button will write the comment to Parameter. A list of all the preliminary modifications can be printed by clicking the Print button.

If preliminary modifications that were added Ad-hoc are available in a previous EAF database then these can be reused (so long as data for the reaction in Parameter have not been significantly changed), saving a great deal of effort. To do this click the Reaction data|Process Ad-hoc preliminary modifications… menu item that displays the Process Ad-Hoc Preliminary modifications window shown in Figure 108. The database to be used is shown, this is the same as the one selected when comparing with an External database (see page 137). Before use it is necessary to click the Check button to ensure that the External Parameter database is sufficiently recent (the Kind and Status fields must be present). By default the All radio button is selected. If the database can be used then the Process button is enabled. Clicking this will add all possible Ad-Hoc preliminary modifications to the Internal Parameter database. Any that cannot be added are listed in the window. This list can be copied to the clipboard by clicking the Copy button or printed by clicking the Print button. The reactions can be investigated individually and further preliminary modifications added as necessary.

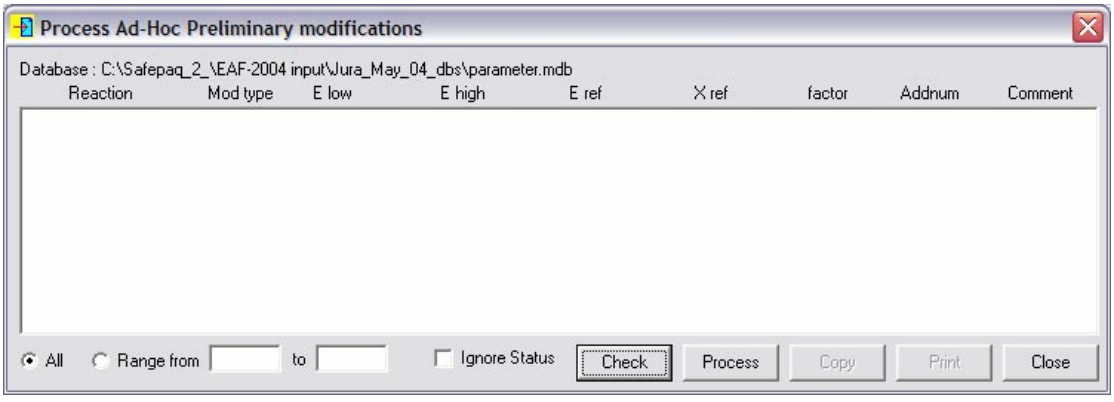


Figure 108. The Process Ad-Hoc Preliminary modifications window.

Rather than process all the Ad-hoc preliminary modifications it is possible to select a range. If the *PreModification* and *PreModSummary* tables in the Parameter database are examined using Access the required Mod numbers can be chosen. The Range from radio button is clicked and the starting and finish modifications (inclusive) are entered in the

text boxes. In some cases the Status of the reaction is unimportant (if experimental data or the data source have been changed in Parameter then the Status field is changed from 0 to 1 and the pre-modification is not added). To ignore the reaction Status check the Ignore Status check box.

It is possible that following the addition of Ad-hoc pre-modifications that for some reactions there may exist redundant Mod type 17 pre-modifications. These should be removed and this can be done by clicking the Reaction data|Find reactions with incorrect ModType 17 pre-modifications… menu item that displays the Reactions with incorrect ModType 17 pre-modifications window shown in Figure 109. Clicking the Get reactions button lists the reactions. If any reactions are shown then select one and click the View data button to open the Reaction data window (Figure 66) where the data can be inspected.

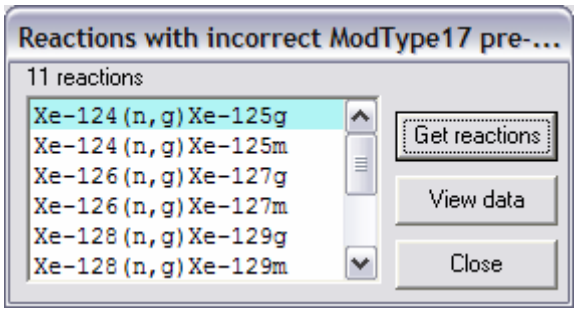


Figure 109. The Reactions with incorrect ModType 17 pre-modifications window.

The major difference for an extended energy library is that data are required between 20 and 60 MeV. A large number of reactions have been added from TALYS using the Add new reactions window (Figure 99), but those already present in say, EAF-2003, need to be extended to 60 MeV. This can be done automatically using data from TALYS by clicking the Reaction data|Find all high-energy data merge pre-modifications|Find all >20 MeV data merge (TALYS) pre-modifications… menu item. This searches through the reaction list and for each reaction with no data > 20 MeV checks if such data exist in TALYS. If so then the data are extracted, scaled by a factor f so that there is no discontinuity at 20 MeV and then stored as a Mod type 13 pre-modification.

For the preparation of the EAF-2007 deuteron-induced library it was necessary to extend a set of reactions above 50 MeV. This was done by clicking the Reaction data|Find all high-energy data merge pre-modifications|Find all >50 MeV data merge (TALYS) pre-modifications… menu item.

For reactions where the threshold is close to 20 MeV the factor required to smoothly join the TALYS data to the existing data at 20 MeV may be significantly different from 1. Such reactions may be better represented by changing the data source to TALYS over the entire energy range. To view the values of the factors click the Reaction data|View High energy factors… menu item, that displays the View High energy factors window shown in Figure 110. Enter the factor required in the text box and click the Get reactions button to list the reactions, the data source and factor (*f*). By default the All sources check box is ticked. This means that even if the existing data comes from TALYS then the reaction is listed (this can occur if the TALYS data < 20 MeV were modified). To remove reactions with a TALYS data source from the data grid, clear the check box.

In order to view the data for a particular reaction click the Visualisation button (which is enabled once a reaction is selected), this copies the selected reaction's data to the Cache (if these are not already present) and displays the Targets and sources window (Figure 63) with the appropriate target and reaction selected. It is then possible to plot the data in the normal manner.

If a reaction already has a data merge pre-modification prior to the automatic data merge with TALYS, then the calculated factor is almost certainly incorrect. For such reactions the calculated factor is replaced with the value 1.0E6. Any reactions with this factors in the table should be investigated.

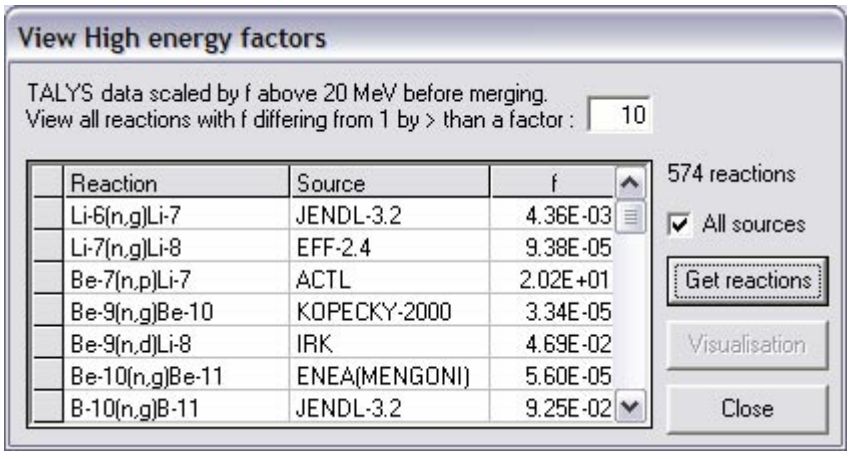


Figure 110. The View High energy factors window.

The change of data source to TALYS for reactions with large factors can be done automatically by clicking the Reaction data|Change data source to TALYS for all reactions with large f menu item. This finds all reactions where $f > 100$ and the data source is not TALYS and then changes it to TALYS

data from the data source given in the Version of TALYS text box in the Settings window (Figure 1).

In the discussion of the Preliminary modifications window (Figure 106) the purpose of the Switch button was given. In order to identify reactions with multiple Mod type 13 modifications click the Reaction data|Find reactions with multiple data merges… menu item, this displays the Reactions with multiple data merges window shown in Figure 111. Each reaction can then be investigated in turn.

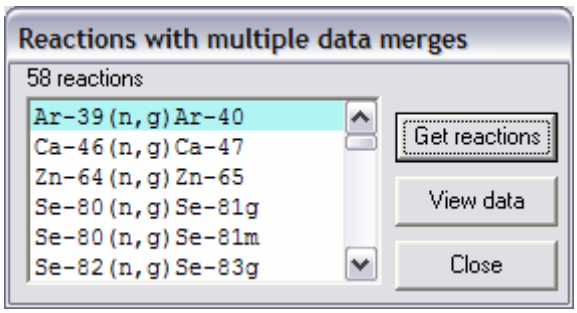


Figure 111. The Reactions with multiple data merges window.

To check which reactions have been extended by a data merge with TALYS data click the Reaction data|Find reactions from TALYS with a data merge… menu item. This displays the Reactions from TALYS with a data merge window which is the same as Figure 111 except that the caption is different.

The TALYS data source may not contain high energy cross section data for all reactions in the EAF project. A second source of data up to 60 MeV is from the IEAF-2001 library. In order to use this data source automatically for any reactions not already completed by data from TALYS click the Reaction data|Find all high-energy data merge pre-modifications|Find all >20 MeV data merge (IEAF) pre-modifications… menu item. This searches through the reaction list and for each reaction with no data > 20 MeV checks if such data exist in IEAF-2001. If so then the data are extracted, scaled by a factor f so that there is no discontinuity at 20 MeV and then stored as a Mod type 13 pre-modification.

Once the collection of pre-modifications is complete, these can be implemented by generating the Final database. This is done by clicking the Reaction data|Generate Final database using preliminary mods menu item. If Final already contains data then a confirmation dialog similar to that shown in Figure 105 is displayed prior to deleting any data. Generating Final involves copying all the data from Master to Final and then implementing the pre-modifications. It takes a reasonably short time (~ 10 mins) to carry out this step.

It is now possible to find the main set of modifications. These are generated by comparing data for each reaction in Final with information in Parameter. Although it is possible to find these modifications in a series of steps using items on the Reaction data|Find modifications sub-menu, it is preferrable to automate this by clicking on the Reaction data|Automate processing… menu item or the twenty-sixth toolbar button. This displays the Automate processing window shown in Figure 112.

The window shows a series of steps, the required ones should be checked. The first step opens the Compact databases window (Figure 4), step 4 refers to the pre-modifications discussed above. If the various steps are to be carried out un-supervised then the Interactive confirmations check box should be unchecked. This stops any confirmation dialogs that require user interaction.

It can be seen that eight modification steps are checked in Figure 112, these are described below. Note that in all cases the flags (Use B and Use R), stored with the experimental data, determine if the data are used to create the modifications.

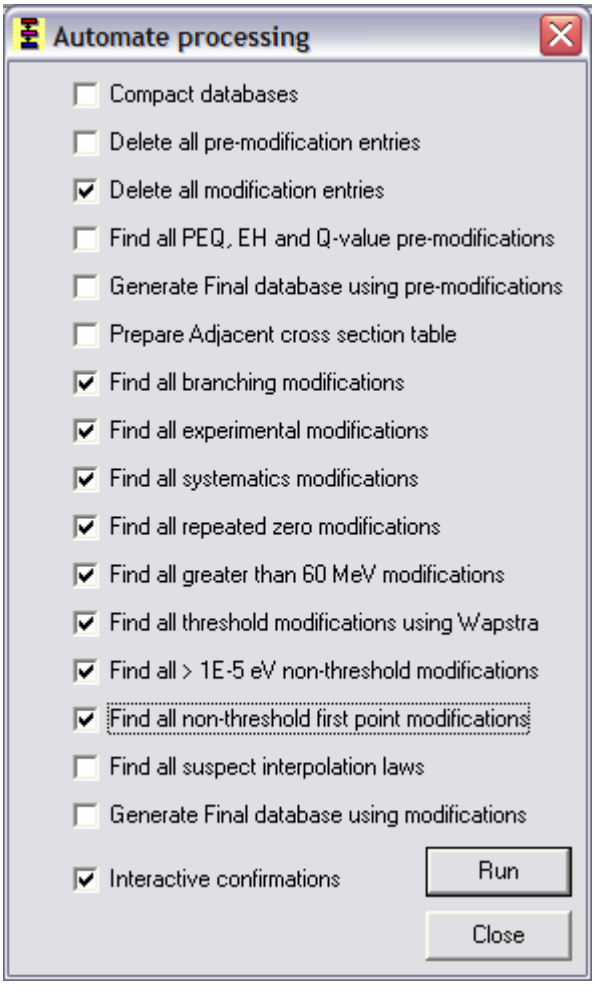

Automate processing
Compact databases
Delete all pre-modification entries
Delete all modification entries
Find all PEQ, EH and Q-value pre-modifications
Generate Final database using pre-modifications
Prepare Adjacent cross section table
Find all branching modifications
Find all experimental modifications
Find all systematics modifications
Find all repeated zero modifications
Find all greater than 60 MeV modifications
Find all threshold modifications using Wapstra
Find all > 1E-5 eV non-threshold modifications
Find all non-threshold first point modifications
Find all suspect interpolation laws
Generate Final database using modifications
Interactive confirmations
Run
Close

Figure 112. The Automate processing window.

Find all branching modifications

(Reaction data|Find modifications|Find all branching modifications) considers first the threshold and then the non-threshold reactions. For each of the threshold reactions the following steps are considered:

1. Are there experimental data for this final state and the other (for a multiplicity = 2 reaction)? If so then calculate the branching ratio at the given energy and store a Mod type 4.
2. Are there experimental data for this final state and the other two (for a multiplicity = 3 reaction)? If so then calculate the branching ratio at the given energy and store a Mod type 4.
3. Are there experimental data points for two final states but not the required final state (e.g. m and Total may be present allowing g to be calculated)? If so then calculate the branching ratio at the given energy and store a Mod type 4.
4. Are there experimental data points for three final states but not the required final state (e.g. g, m and Total may be present allowing n to be calculated)? If so then calculate the branching ratio at the given energy and store a Mod type 4.
5. Remaining branching ratios by systematics, storing a Mod type 4.

For non-threshold reactions the following steps are considered:

1. Are there experimental data at 0.0253 eV for this final state and the other (for a multiplicity = 2 reaction)? If so then calculate the branching ratio at the energy and store a Mod type 4.
2. Are there experimental data at 0.0253 eV for this final state and the other two (for a multiplicity = 3 reaction)? If so then calculate the branching ratio at the energy and store a Mod type 4.
3. Are there experimental data points at 0.0253 eV for two final states but not the required final state (e.g. m and Total may be present allowing g to be calculated)? If so then calculate the branching ratio at the given energy and store a Mod type 4.
4. Are there experimental data points at 0.0253 eV for three final states but not the required final state (e.g. g, m and Total may be present allowing n to be calculated)? If so then calculate the branching ratio at the given energy and store a Mod type 4.
5. Remaining branching ratios at thermal energies by systematics, storing a Mod type 4.

6. Are there experimental resonance integral data for this final state and the other (for a multiplicity = 2 reaction)? If so then calculate the branching ratio and store a Mod type 4.
7. Are there experimental resonance integral data for this final state and the other two (for a multiplicity = 3 reaction)? If so then calculate the branching ratio and store a Mod type 4.
8. Are there experimental resonance integral data for two final states but not the required final state (e.g. m and Total may be present allowing g to be calculated)? If so then calculate the branching ratio and store a Mod type 4.
9. Are there experimental resonance integral data for three final states but not the required final state (e.g. g, m and Total may be present allowing n to be calculated)? If so then calculate the branching ratio and store a Mod type 4.
10. Remaining branching ratios in the mid-range use those calculated at thermal energy.
11. Are there experimental data at 14.5 MeV for this final state and the other (for a multiplicity = 2 reaction), if so then calculate the branching ratio at the given energy and store a Mod type 6.
12. Are there experimental data at 14.5 MeV for this final state and the other two (for a multiplicity = 3 reaction), if so then calculate the branching ratio at the given energy and store a Mod type 6.
13. Are there experimental data points at 14.5 MeV for two final states but not the required final state (e.g. m and Total may be present allowing g to be calculated)? If so then calculate the branching ratio at the given energy and store a Mod type 6.
14. Are there experimental data points at 14.5 MeV for three final states but not the required final state (e.g. g, m and Total may be present allowing n to be calculated)? If so then calculate the branching ratio at the given energy and store a Mod type 6.
15. Remaining branching ratios at 14.5 MeV by systematics, storing a Mod type 6.

Details about the definition of branching ratios are given in Appendix 4.

Find all experimental modifications

(Reaction data|Find modifications|Find all experimental modifications) carries out renormalisation to experimental data for all the reactions, storing a Mod type 3.

Find all systematics modifications

(Reaction data|Find modifications|Find all systematics modifications) carries out renormalisation to systematic values for all the reactions, storing a Mod type 2.

Find all repeated zero modifications

(Reaction data|Find modifications|Find all repeated zero modifications) finds reactions where there is more than one zero cross section at the start of the data. These additional points are removed using a Mod type 8 modification.

Find all greater than 60 MeV modifications

(Reaction data|Find modifications|Find all greater than 60 MeV modifications) finds reactions where there are data points with energies greater than 60 MeV. These unnecessary points are removed using a Mod type 5 modification. In non-extended libraries the menu item shows 20 MeV.

Find all threshold modifications using Wapstra

(Reaction data|Find modifications|Find all threshold modifications using Wapstra) compares the threshold in the file with that calculated using the Wapstra mass table. If Abs($Q_{Wapstra}$ - Q_{file}) > 10000 eV, then a modification is stored as Mod type 7.

Find all > 1 E-5 eV non-threshold modifications

(Reaction data|Find modifications|Find all > 1E-5 eV non-threshold modifications) finds the reactions which are non-threshold, and where the first point is in the range 1 x 10^{-5} < E < 1 eV. For these reactions add a new point at 1 x 10^{-5} eV, storing the modification as Mod type 8.

Find all non-threshold first point modifications

(Reaction data|Find modifications|Find all non-threshold first point modifications) finds the reactions which are non-threshold, and where the first energy value is either < 1 x 10^{-5} (in practice this means E = 0) or > 1000 eV or E = 1 x 10^{-5}eV, but cross section = 0. For these reactions the first point is changed to Energy = 1 x 10^{-5} eV and cross section = 1 x 10^{-10} b, the interpolation law between points 1 and 2 is changed to 1 if necessary. These two modification are stored as Mod type 8 and Mod type 10.

All the above modifications can be found automatically. The remaining modifications involve changes to the interpolation law data, but these require user interaction. The first step is to generate a table of data points for non-threshold reactions where there is a significant gap (E_i / E_{i-1} > 1.5) between data

points (exclude reactions starting with $E = 0$). This is done by clicking the Reaction data|Prepare Adjacent cross section table menu item or the sixth check box in Figure 112. Then using this table a set of suspect reactions is found by clicking the Reaction data|Find modifications|Find all suspect interpolation laws sub-menu item or ticking the fifteenth check box in Figure 112.

A reaction is suspect if the ratio of energies > 2 and the interpolation law is not 5 or 1. These suspect reactions can be viewed in the Interpolation law modifications window shown in Figure 113, this is displayed by clicking the Reaction data|Find modifications|Find interpolation law modifications manually… sub-menu item. Note that at the same time the Targets and sources window (Figure 63) also opens, as the two windows are used together.

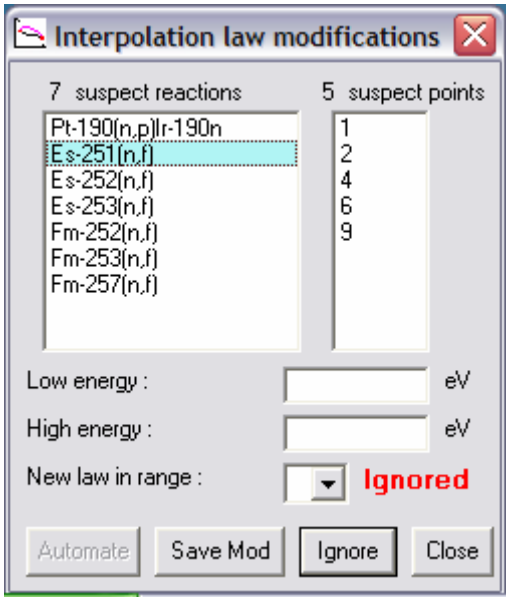


Figure 113. The Interpolation law modifications window.

The Interpolation law modifications window shows the suspect reactions in the list box, and when one is selected the number of suspect points and their point numbers are shown. At the same time data for this reaction are copied to the Cache (if they are not already present), and the target and reaction are selected in the Targets and sources window. From here it is possible to plot the data in the usual way and decide if there is a need to modify the interpolation law. If the law is correct, then click the Ignore button in Figure 113; the window shows this (by the word 'Ignored') and the status is stored in the database. However, if some of the data points do require law changes then select these points in the Data visualisation window (Figure 64), these points are also selected in the Reaction data window (Figure 66). The high and low points of the selected

data are then also shown in the text boxes in Figure 113. Select a new law in the dropdown list and click the Save Mod button to add a new modification. Note that the confirmation dialog shown in Figure 114 is displayed before the modification is saved.

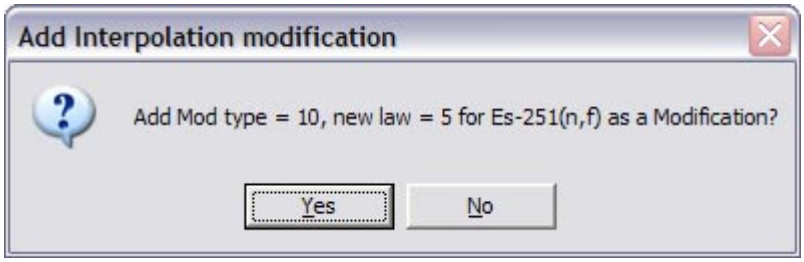


Figure 114. Confirmation dialog prior to adding modification.

As modifications are saved, they are also stored in the *InterpMods* table. If there are any entries in this table (as a result of a previous use of this window) then the Automate button is enabled. Clicking this checks each suspect reaction in turn and if there is an entry for this reaction with the same data source in the *InterpMods* table then the modification data are used to create a new modification (without any confirmation dialog). If the reaction has a different source then it is not treated, and if it is not present in the *InterpMods* table then the 'Ignored' flag is set. When all the suspect reactions have been considered then the list box in Figure 113 shows only the reactions that have not been treated.

The collection of all modifications that have been made can be viewed by clicking the Reaction data|View modifications… menu item or the twenty-fifth toolbar button which displays the Modifications window shown in Figure 115.

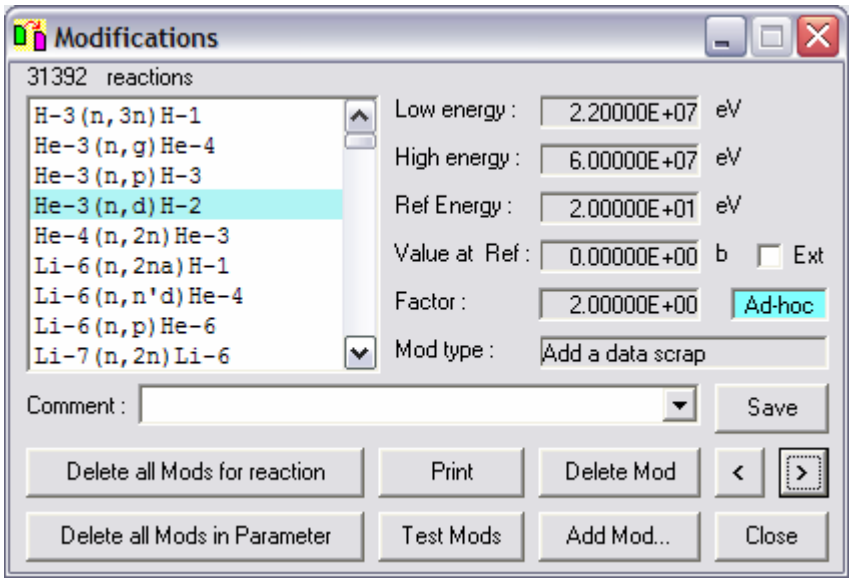


Figure 115. The Modifications window.

The description of this window is exactly the same as following Figure 106. Refer to that text for details. Clicking the Add Mod… button displays the Add modification window shown in Figure 116. Note that if the Shift key is pressed while clicking the Add Mod… button, then the details of the currently selected reaction are added to Figure 116.

Figure 116 is very similar to Figure 107, the differences are that a wider range of modifications are available in the Mod type dropdown list, there is an additional text box to enter a value in the Addnum field and there is a Mid range check box. The latter is required because if the modification refers to the mid-energy range for a non-threshold reaction, then it is necessary to store this value for use in branching calculations. Note that the boxes that require data are shown in white rather than grey. In the case of the $1/v$ addition (mod type 11) modification it is optional to enter values in the Ref. Energy and Value at Ref text boxes. If this is done then the $1/v$ curve will pass through the specified point, otherwise it will pass through the point at High energy.

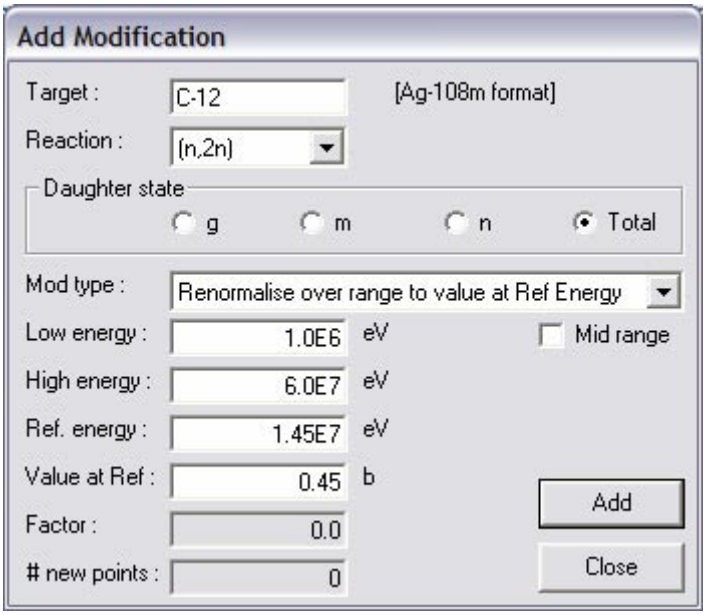


Figure 116. The Add modification window.

If the modification adds a Data scrap (Mod Type 12) then a File name list box and set of Adjust to fit radio buttons are shown (very similar to those in Figure 71). These need to be completed before clicking the Add button.

If modifications that were added Ad-hoc are available in a previous EAF database then these can be reused (so long as data for the reaction in Parameter have not been changed), saving a great deal of effort. To do this click the Reaction data|Process Ad-hoc modifications… menu item that

displays the Process Ad-Hoc modifications window. This is very similar to Figure 108, but displays modifications not preliminary modifications. The database to be used is shown, this is the same as the one selected when comparing with an External database (see page 137). Before use it is necessary to click the Check button to ensure that the External Parameter database is sufficiently recent (the Kind and Status fields must be present). As in the case of pre-modifications a range of Mod numbers can be considered as well as the default of processing all the Ad-hoc modifications. If the database can be used then the Process button is enabled. Clicking this will add all possible Ad-Hoc modifications to the Internal Parameter database. Any that cannot be added are listed in the window. This list can be copied to the clipboard by clicking the Copy button or printed by clicking the Print button. The reactions can be investigated individually and further modifications added as necessary.

It is possible that following the addition of Ad-hoc modifications, that for some reactions there may exist redundant Mod type 17 modifications. These should be removed and this can be done by clicking the Reaction data|Find reactions with incorrect ModType 17 modifications… menu item that displays the Reactions with incorrect ModType 17 modifications window which is identical to Figure 109, except that the title is different. Clicking the Get reactions button lists the reactions. If any reactions are shown then select one and click the View data button to open the Reaction data window (Figure 66) where the data can be inspected.

Once the collection of modifications is complete, these can be implemented by generating the Final database. This is done by clicking the Reaction data|Generate Final database using modifications menu item. Final already contains data, but these are not deleted, only further changed using the modifications. The time taken to carry out this step depends on the total number of modifications, but is typically about 8 mins.

The assembling of all reaction data is now complete. The next steps are a series of iterations to view, check and correct the data to ensure that no further modifications are required. Twenty tests on the data in Final can be carried out. The first check is to ensure that no negative cross section data have been produced during the production of Final. To check this click the Reaction data|Test Final for|Negative cross sections… submenu item, this displays the Negative cross sections window shown in Figure 117.

To check if there are any reactions with negative cross sections, click the Get reactions button, this takes about 20 s to check all the data. If, as required, there are no reactions shown then the check is complete. If any reactions are shown then select one and click the View data button to open the Reaction data window (Figure 66) where the data can be inspected.

The second test shows if any reactions have zero cross section at high energy. To check this click the Reaction data|Test Final for|Missing high energy data… submenu item, this displays the Missing high energy data window which is identical to Figure 117 except for the caption.

The third test shows if any reactions have negative energy values. To check this click the Reaction data|Test Final for|Negative energies… submenu item, this displays the Negative energy values window which is identical to Figure 117 except for the caption.

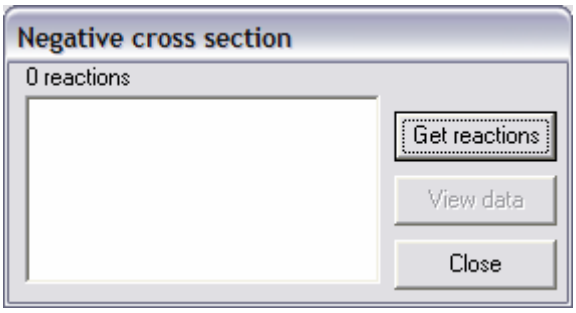


Figure 117. The Negative cross sections window.

The fourth test shows if any non-threshold reactions have the first energy point ≠ 1 x 10^{-5} eV. To check this click the Reaction data|Test Final for|Non-threshold reactions with E<>1E-5 eV… submenu item, this displays the Non-threshold reactions with E<>1E-5 eV window which is identical to Figure 117 except for the caption.

The fifth test shows if any non-threshold reactions have any data points with cross section = 0. To check this click the Reaction data|Test Final for|Non-threshold reactions with any xs=0… submenu item, this displays the Non-threshold reactions with any xs=0 window which is identical to Figure 117 except for the caption.

The sixth test shows if any threshold reactions have other than the first data points with cross section = 0. To check this click the Reaction data|Test Final for|Threshold reactions with other than 1st point xs=0… submenu item, this displays the Non-threshold reactions with other than 1st point xs=0 window which is identical to Figure 117 except for the caption. Note that if reactions are shown in the list box, then it may be possible to generate a set of modifications to correct them by

clicking on the Reaction data|Find all 2nd type of repeated zero modifications menu item. This finds reactions where the first two points have cross section = 0 and replaces the second value with a value linearly interpolated from the first and third points. Usually this class of modifications will not be required.

The seventh test shows if any reactions have the data point at 60 MeV missing. To check this click the Reaction data|Test Final for|Missing 60 MeV data point… submenu item, this displays the Missing 60 MeV data point window which is identical to Figure 117 except for the caption. Note that if reactions are shown in the list box, then it may be possible to generate a set of modifications to correct them by clicking on the Reaction data|Find all missing 60 MeV modifications menu item. This finds reactions where there is no data point at 60 MeV and adds it using a value linearly extrapolated from the last two data points. Usually this class of modifications will not be required. For non-extended libraries, 20 replaces 60 on all menu items.

The eighth test shows if any reactions contain repeated energy points. To check this click the Reaction data|Test Final for|Repeated energy points… submenu item, this displays the Reactions with repeated energy points window which is identical to Figure 117 except for the caption. Note that if reactions are shown in the list box, then it is possible to correct them by clicking on the Reaction data|Remove repeated energy points from Final menu item. This step is described later.

The ninth test shows if any reactions contain inconsistent interpolation ranges. It is possible that the number of interpolation ranges for a reaction shown in the *Reaction* and *Interpolation* tables of Final may not agree. To check this click the Reaction data|Test Final for|Inconsistent Interpolation ranges… submenu item, this displays the Reactions with inconsistent Interpolation ranges window which is identical to Figure 117 except for the caption.

The tenth test shows if any reactions contain inconsistent cross section data. It is possible that the number of data points for a reaction shown in the *Reaction* and *Cross section* tables of Final may not agree. To check this click the Reaction data|Test Final for|Inconsistent Cross section data… sub-menu item, this displays the Reactions with inconsistent Cross section data window which is identical to Figure 117 except for the caption.

The eleventh test shows if any reactions contain inconsistent numbers of data points. It is possible that the number of data points or ranges for a reaction shown in the *Reaction, Cross*

section and *Interpolation* tables of Final may not agree. To check this click the Reaction data|Test Final for|Inconsistent number of data points… submenu item, this displays the Reactions with inconsistent number of data points window which is identical to Figure 117 except for the caption.

The twelfth test shows if any threshold reactions contain a first point with energy < 1eV. To check this click the Reaction data|Test Final for|Threshold reactions with wrong 1st point… submenu item, this displays the Theshold reactions with wrong 1st point window which is identical to Figure 117 except for the caption.

The thirteenth test shows if any threshold reactions contain a first range with a interpolation law that uses the log of the cross section (laws 4 or 5). Since the first data point has cross section = 0, such a law would cause a crash. To check this click the Reaction data|Test Final for|Threshold reactions with wrong 1st law… submenu item, this displays the Theshold reactions with wrong 1st law window which is identical to Figure 117 except for the caption.

The fourteenth test only applies to libaries with energies > 20 MeV. For such libraries all reactions should contain data above 20 MeV. To check this click the Reaction data|Test Final for|Missing data above 20 MeV… submenu item, this displays the Missing data above 20 MeV window which is identical to Figure 117 except for the caption.

The fifteenth test shows if any reactions have data points with energies > 60 MeV. To check this click the Reaction data|Test Final for|Data points > 60 MeV… submenu item, this displays the Data points > 60 MeV window which is identical to Figure 117 except for the caption. For non-extended libraries, 20 replaces 60 on the menu item.

The sixteenth test shows if any reactions have a Q-value of zero. To check this click the Reaction data|Test Final for|Q value = 0… submenu item, this displays the Q value = 0 window which is identical to Figure 117 except for the caption.

The seventeenth test actually uses data in Parameter, but devived from Final. A systematic formula for the total non-elastic cross sections is available [10]. The sum of the cross sections for all the reactions at 14.5 MeV should agree closely with the non-elastic systematic for this energy. Any reactions which differ by more than a factor of 2 need further investigation. To check this click the Reaction data|Test Final for|Inconsistent non-elastic data at 14.5 MeV… sub-menu item, this displays the Inconsistent non-elastic data at

14.5 MeV window which is identical to Figure 117 except for the caption.

The eighteenth test is identical to the seventeenth except that data at 40 MeV are considered. To check, click the Reaction data|Test Final for|Inconsistent non-elastic data at 40.0 MeV… submenu item, this displays the Inconsistent non-elastic data at 40.0 MeV window which is identical to Figure 117 except for the caption.

The nineteenth test shows if any reactions have energies for the first and second data points that are not increasing. To check this click the Reaction data|Test Final for|Wrong energy order for points 1 and 2… submenu item, this displays the Wrong energy order for points 1 and 2 window which is identical to Figure 117 except for the caption.

The twentieth test shows if any reactions have a very sharp discontinuity in cross section as the energy increases. Such a steep gradient can cause problems when the group cross sections are calculated. To check this click the Reaction data|Test Final for|Very steep gradient… submenu item, this displays the Reactions with very steep gradient window which is identical to Figure 117 except for the caption.

A new feature in EASY-2003 was the addition of a Quality score for each reaction. This score indicates whether there are any differential or integral experimental data and whether the data agree with the EAF library. Table 3 shows the definitions of the scores.

Table 3. EAF-2007 Quality scores.

Score	Description
0	No experimental data exists
1	Limited differential data which disagrees with the library (weak disagreement)
2	Limited differential data which agrees with the library (weak agreement)
3	Differential data which disagrees with the library (strong disagreement)
4	Differential data which agrees with the library (strong agreement)
5	Both differential and integral data exist or only integral data exist and these are not in agreement with the library
6	Both differential and integral data exist and they are in agreement with the library (validation)

The Quality scores for reactions can be viewed by clicking the Reaction data|Quality scores… menu item which displays the Quality scores window shown in Figure 118. A choice of reactions to view is made by selecting one of the radio buttons

in the View reactions group and clicking the Get reactions button. The number of reactions is indicated at the top right of the window.

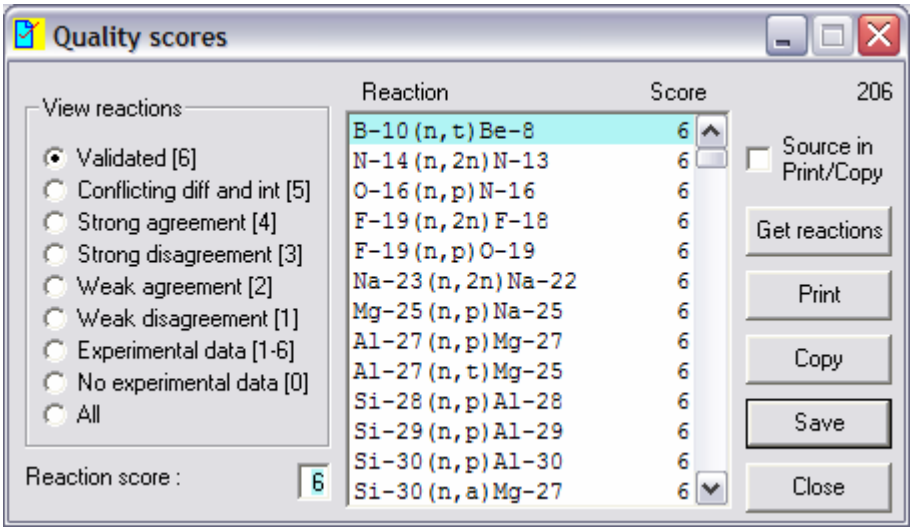


Figure 118. The Quality scores window.

Selecting a reaction displays the score in a text box enabling it to be changed. Clicking the Save button saves the change. Note that if all reactions (or those with score 0) are displayed then for high mass targets the new score is not displayed in the list. This technical problem can be avoided by changing scores with one of the other reaction radio buttons clicked. The list of reactions can be copied to the clipboard by clicking the Copy button or printed by clicking the Print button. Clicking the Close button closes the window.

The data source of the selected reaction is displayed as a ToolTip when the cursor hovers over the Reaction listbox. This information can be included when reactions are copied or printed if the Source in Print/Copy option is checked.

During the review of data in Final, it may be necessary to follow all the above processing steps for a single reaction to improve the data. This can be done by clicking the Reaction data|Single reaction processing… menu item or the twenty-seventh toolbar button which displays the Single reaction processing window shown in Figure 119. This consists of a series of tabs which divide the processing into a number of phases. The window opens with the Source tab displayed. Clicking on the Get reactions button will show all the targets in the first list box, selecting one of these displays the reactions for the target in the second list box. The selected reaction name is shown in the window's title bar.

Note that the Get reactions button is only enabled if the Final database has been constructed. To avoid having to click the Get

reactions button each time the window is opened (provided that Final has been constructed), the window will open with the reactions already displayed if the Auto open Single Reac check box is ticked in the Settings window (Figure 1). An additional feature that saves time when selecting reactions has been added from EASY-2005. The window will open with the target and reaction selected that were used when the window was closed previously.

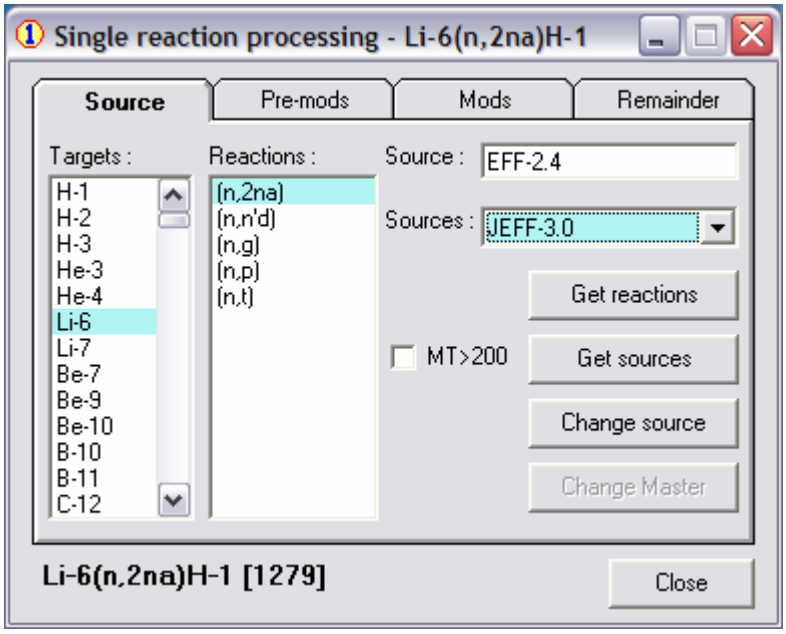


Figure 119. The Single reaction processing window (Tab 1).

Note that if a reaction is split into several final states then these must be considered consecutively (g, then m, then n) without shutting down SAFEPAQ-II, so that the systematics data in the various Summary tables in Parameter can be correctly stored.

Note that the selected reaction and the reaction number are also displayed at the bottom left of the window. This is necessary as in some cases the entire reaction including the daughter cannot be displayed in the window caption.

Note that only sources relevant to the specified type of incoming particle are displayed.

Click the Get sources button to enter all the sources for the selected reaction into the dropdown list box. Note that sources with the selected reaction's final state or 99 are shown, this enables the source of a split reaction to be changed to a source which only contains the total cross section. If it is necessary to use summed data from a data source, then the MT>200 check box must be checked so that this data source is available in the dropdown list. The current source can be altered by clicking one of the sources in the dropdown list. To make the change click the Change source button. Before data are changed in

the Parameter database the confirmation dialog shown in Figure 120 is displayed. If the source has been changed then click on the Change Master button to change data for this reaction in the Master database. Now click on the Pre-mods tab to start the next phase.

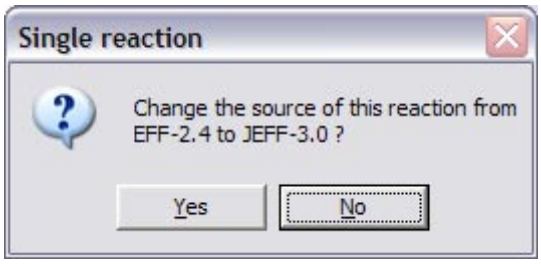


Figure 120. Confirmation dialog prior to changing data source.

Figure 121 shows the window with this tab selected. Text in the window shows the number of pre-modifications that exist for the reaction. If this is greater than 0, then the Delete button is enabled and the existing pre-modifications can be removed. Now click the Find pre-mods button to find any pre-modifications required for the reaction. Note that it is possible to use the existing Pre-modifications by just clicking the Change Final button. As the pre-modification types are considered a tick or a cross is displayed next to the pre-modification description to indicate if it been found. Other pre-modifications (specifically a Data merge) can be entered by clicking the Add pre-mod… button. This displays the Add Preliminary modification window shown in Figure 107. Note that the Target, Reaction and Final state details are already entered. When carrying out a Data merge, the value of E_H is inserted in the Ref. energy text box. In cases where the reaction is split this value is slightly increased to avoid problems. Click the Delete pre-mod… button to show a series of Confirmation dialogs enabling each pre-modification to be deleted in turn. Click the Change Final button to implement these pre-modifications in Final. Click the Change Adjacent button to change the data in the *Adjacent cross section* table for the reaction.

Note that there is a major distinction between clicking the Delete and the Delete pre-mod... buttons. The former removes all the pre-modification for the reactions, while the latter actually adds a Mod type 17 modification to the existing pre-mods. The reason for this is that pre-modifications generated automatically can be removed. Removal of a pre-modification by the use of a Mod type 17 pre-modification is also stored and can be reused in the next EAF project (see discussion on page 84). Now click on the Mods tab to display the third tab shown in Figure 122.

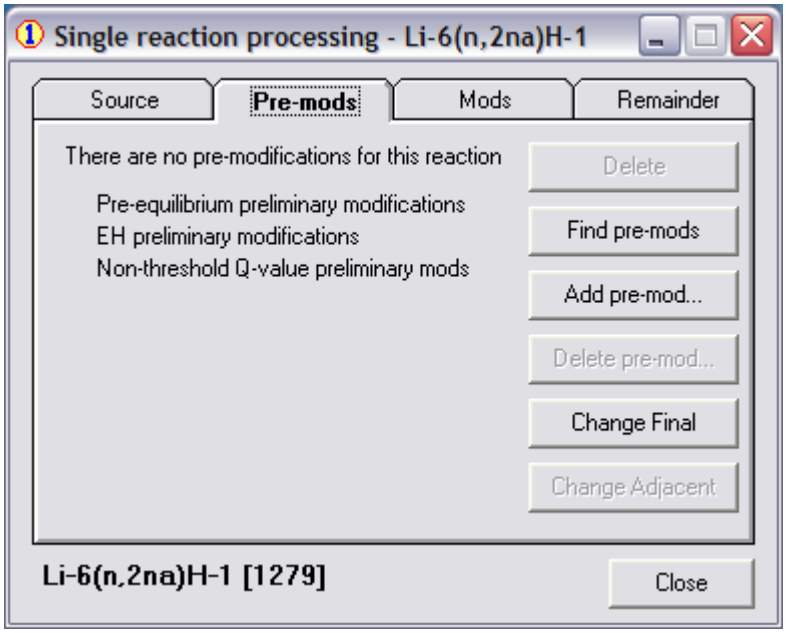


Figure 121. The Single reaction processing window (Tab 2).

Text in the window shows the number of modifications that exist for the reaction. If this is greater than 0, then the Delete button is enabled and the existing modifications should be removed. Note that if required, the existing modifications can be used to recalculate Final. Now click the Find mods button to find any modifications required for the reaction. As the various modification types are considered a tick or a cross is displayed next to the modification description to indicate if modifications have been found. Click the Interp mods… button to open the Interpolation law modifications window (Figure 113) to decide if the interpolation law needs to be changed. Additional modifications can be entered by clicking the Add mod… button. This displays the Add Modification window shown in Figure 116. Note that the Target, Reaction and Final state details are already entered. Click the Delete mod… button to show a series of Confirmation dialogs enabling each modification to be deleted in turn. Click the Change Final button to implement these modifications in Final. The same distinction between deleting all the modifications and deleting one discussed above also applies here. Now click on the Remainder tab to display the fourth tab shown in Figure 123.

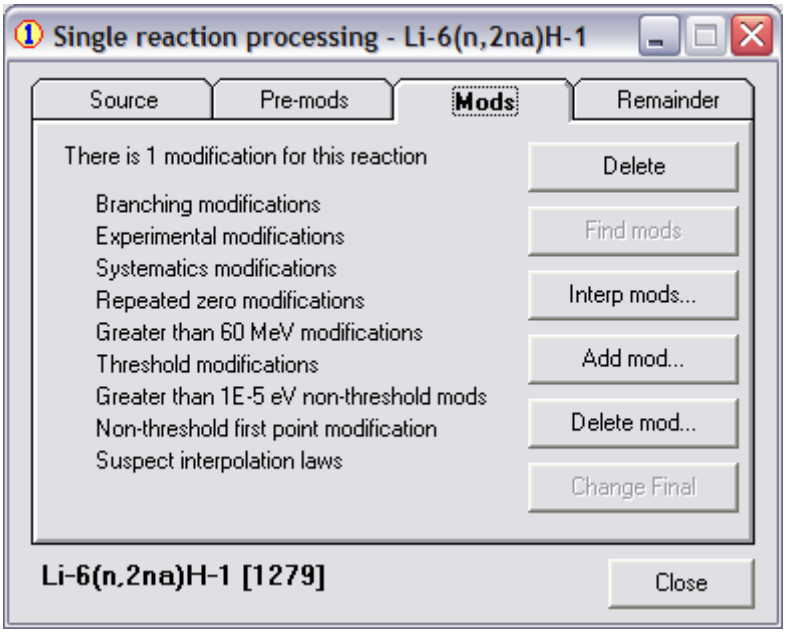


Figure 122. The Single reaction processing window (Tab 3).

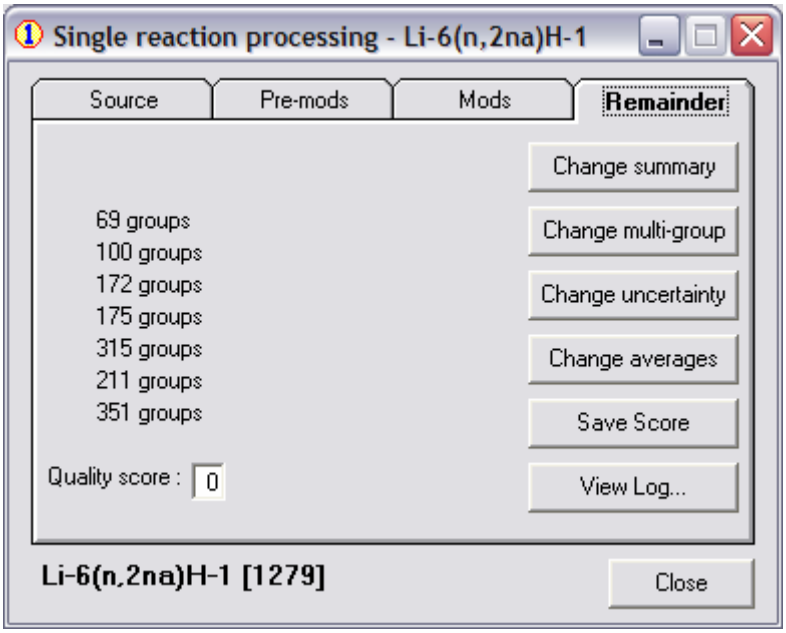


Figure 123. The Single reaction processing window (Tab 4).

Click the Change summary button to change the summary values (discussed below). Click the Change multi-group button to change the multi-group values (discussed below), as each energy group is completed a tick is shown against the group name. Click the Change uncertainty button to change the uncertainty values (discussed below). Click the Change averages button to change the average cross section values in the various neutron spectra values (see page 66). The Quality score for the reaction (see page 103) is displayed, this can be changed and then saved by clicking the Save Score button.

When changes are made it is a good idea to add comments in the Log. This can be done by clicking the View Log… button to open the Log window (Figure 6).

The final processing action for the data in the Final database is to remove any repeated energy points. Reactions where they occur are indicated by the eighth test described on page 100. If there are repeated points then click on the Reaction data|Remove repeated energy points from Final menu item. This step takes typically from a few minutes to 1.5 hours, depending on the number of reactions and replaces a set of points with the same energy by a set separated by a single digit in the sixth decimal place.

It can now be assumed that the data in Final are good enough. The data can now be further processed. Clicking the Reaction data|Generate data|Generate summary of Final database submenu item will start the calculation of the thermal, 30 keV, 14.5 MeV, 20 MeV and resonance integral values for each reaction and put the results in various tables in the Parameter database. Also systematics data for each reaction are stored in tables in Parameter. If summary data already exist then the confirmation dialog shown in Figure 124 is displayed. Generating summary data takes about 3 hours.

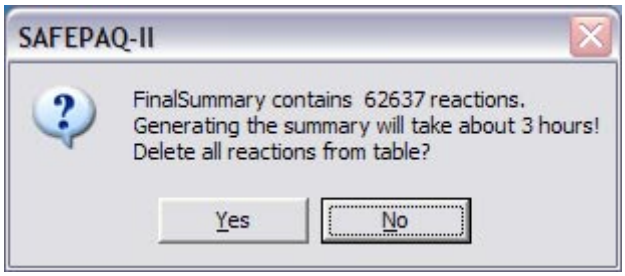


Figure 124. Confirmation dialog prior to changing summary data.

Clicking the Reaction data|Generate data|Generate multi-group data… submenu item will display the Multi-group files window shown in Figure 125. Check the energy groups that need to be calculated, if the elapsed time is required then check the Timer option. Clicking the Calculate button will start the calculation. Since calculating each group structure can take many hours, there is a facility for interrupting the calculation. While the calculation is running, the caption of the second button changes to STOP calculation!. Clicking this will stop the calculation at the end of the next reaction. However, the progress of the calculation is stored and the dialog shown in Figure 126 is displayed next time. Typical calculation times are: 69-groups 6h, 100-groups 10h, 172-groups 14h, 175-groups 16h, 315-groups 36h, 211-groups 15h, 351-groups 25h.

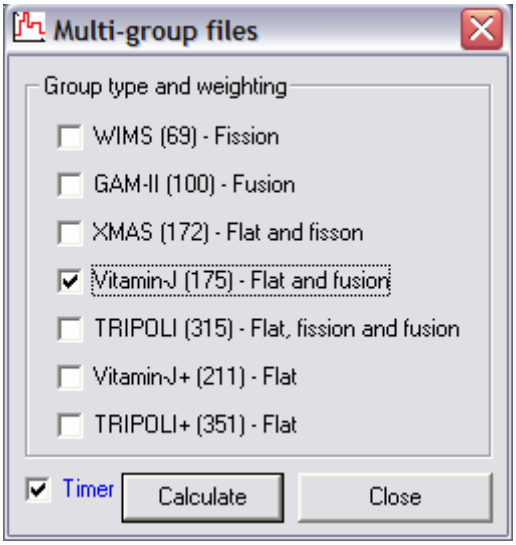


Figure 125. Multi-group files window.

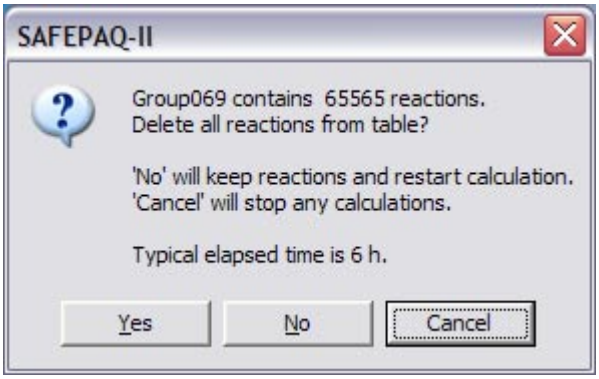


Figure 126. Confirmation dialog prior to starting multi-group calculation.

Figure 126 shows the number of reactions that have already been calculated. Clicking the No button will keep the results and restart the calculation. Clicking Yes will remove existing results and start again. Note that where there is more than one weighting, give the same answer for each confirmation dialog. A mathematical description of the methods of multi-group calculation is given in Appendix 3.

Clicking the Reaction data|Generate data|Generate uncertainty data submenu item will start the calculation of the uncertainty data for all the reactions. If uncertainty data already exist then a confirmation dialog similar to Figure 124 is displayed. This step takes about 5 minutes.

The summary information generated above can be used to carry out validation of the Final data against the experimental and systematic data held in Parameter. Clicking the Reaction data|Validation plots… menu item or the twenty-eighth toolbar button displays the Validation plots window shown in Figure 127. Since EASY-2005, three distinct types of graphs can be plotted. First consider the histogram plots, selected by clicking the Histogram radio button.

Select a reaction in the dropdown list box, a comparison type (C/S shows the Final/Systematics ratio, C/E shows the Final/Experimental ratio and C/T shows the Final/Trend ratio). The C/T option is disabled when the Validation plots window is opened from the menu or Toolbar. The use of this option is described in the Analysis section. From EAF-2007 the cross section analysis feature discussed later enables trend lines to be stored, and these can also be used for validation. Check one or more of the Final state options (more than one final state results in multiple graphs) and the required energy. An additional feature from EASY-2005 is the ability to produce C/S plots at 20 MeV for some reactions. Note that if the Include summed data with Total check box is ticked then comparison is made with experimental data for the total cross section and the sum of all final states for split reactions. These summed reactions are not actually present in the Final database. Clicking the Plot button displays the Validation plot window shown in Figure 128.

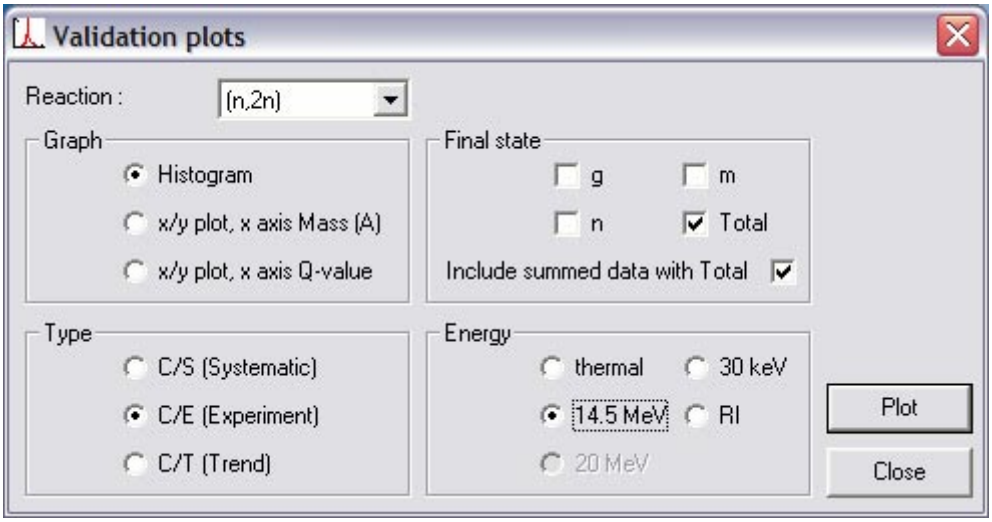


Figure 127. Validation plots window.

Figure 128 shows the C/E data plotted as a histogram. In order to see which reactions are responsible for the scatter about the ideal value of 1.0, click on the graph at a vertex of the histogram and the Validation data window shown in Figure 129 is displayed. This shows the reactions that have C/E values in the selected range. Select a reaction and the data from Final (for summed data the reactions are not in Final) and for the experiment (or from systematics) are displayed. The exact C/E value is also shown. This is necessary because the summary data are for energies of 25.3 meV, 30 keV, 14.5 MeV and 20 MeV. If the experimental data are not exactly at these energies, then the exact C/E (calculated using interpolation where necessary) may differ from the value shown in the list box. The thickness of the histogram line can be altered by clicking on the

Options|Thick lines menu item (this option has been selected in Figure 128).

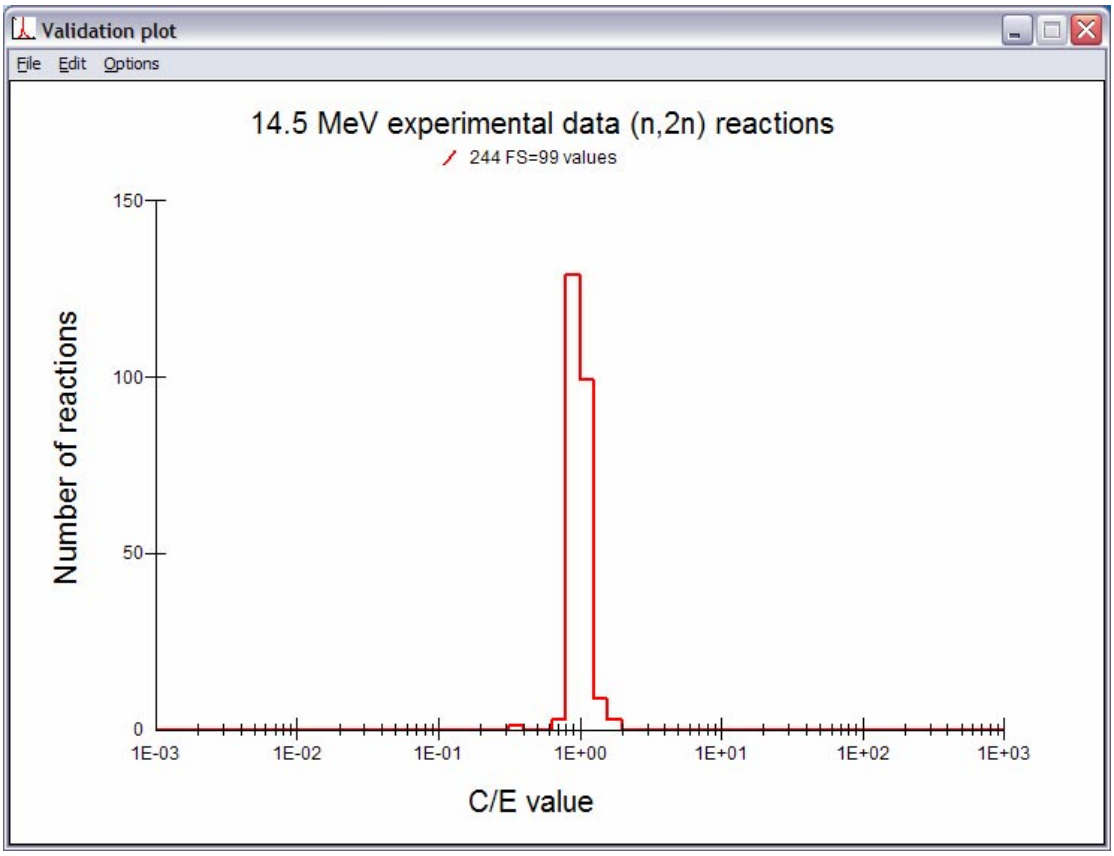


Figure 128. Validation plot window.

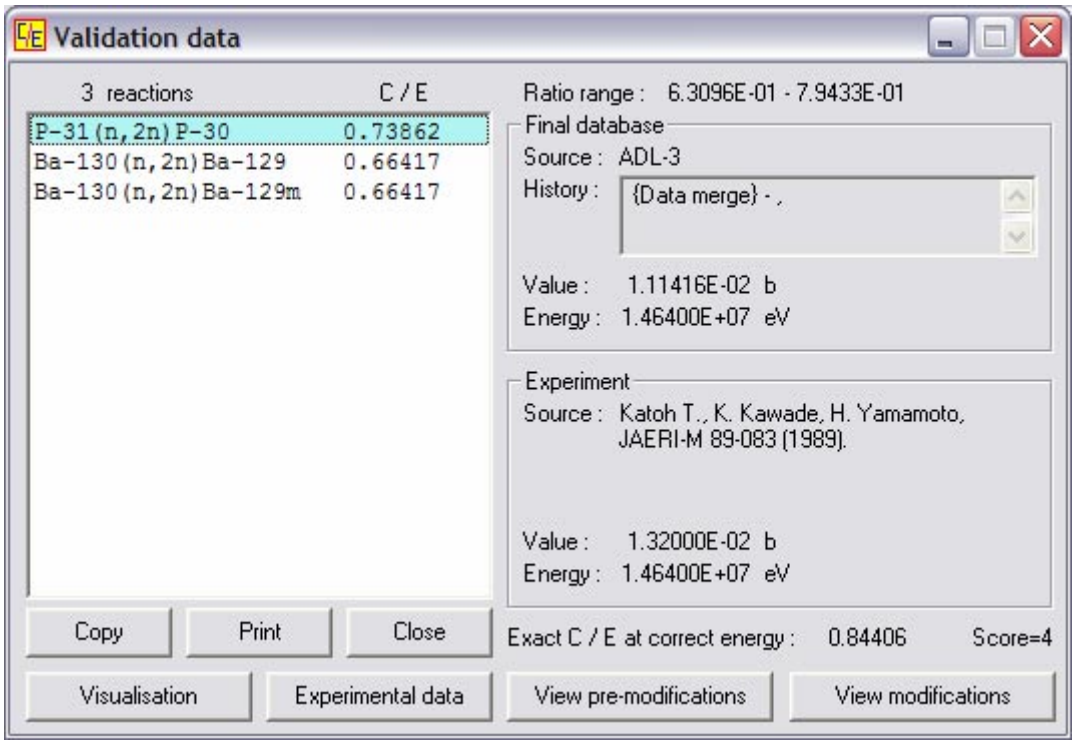


Figure 129. Validation data window.

Figure 129 can be used to investigate reactions with discrepant C/E values. Clicking the Visualisation button copies the selected reaction's data to the Cache (if these are not already present) and displays the Targets and sources window (Figure 63) with the appropriate target and reaction selected. It is then possible to plot the data in the normal manner.

Clicking the Experimental data button will open the appropriate Experimental data window (Figure 29 - Figure 34) and select the correct target. It is then possible to either change which experimental data are used or to add another entry.

Clicking the View pre-modifications button will open the Preliminary modifications window (Figure 106) so that these can be checked. Because it is likely that no pre-modifications exist for the reaction, no attempt is made to select the correct reaction.

Clicking the View modifications button will open the Modifications window (Figure 115) so that these can be checked. Because it is possible that no modifications exist for the reaction, no attempt is made to select the correct reaction.

The Quality score for the reaction is shown and it is possible to print or copy to the clipboard all the listed reactions by clicking the Print or Copy buttons respectively.

In Figure 128 it is possible to print or copy the plot to the clipboard by clicking the File|Print or Edit|Copy menu items respectively.

Returning to Figure 127, the second type of plot, that of C/E or C/S as a function of target mass (A) can be made by selecting the x/y plot, x axis Mass (A) radio button. Select the other options as in the case of a histogram, then clicking the Plot button displays the Validation plot (A) window shown in Figure 130.

Figure 130 shows the C/E data plotted as a function of atomic mass. In order to identify the various points click on one to see details presented in the status bar of the main window. It is possible to print or copy the plot to the clipboard by clicking the File|Print or Edit|Copy menu items respectively. The appearance of the graph can be altered; clicking the Options|Y axis menu item displays a submenu with five entries allowing the y axis range to be selected. In Figure 130 the option E-1 – E1 has been checked. Clicking the Options|X axis menu item displays a submenu with three entries allowing the x axis range

to be selected. In Figure 130 the option 0 - 250 has been checked.

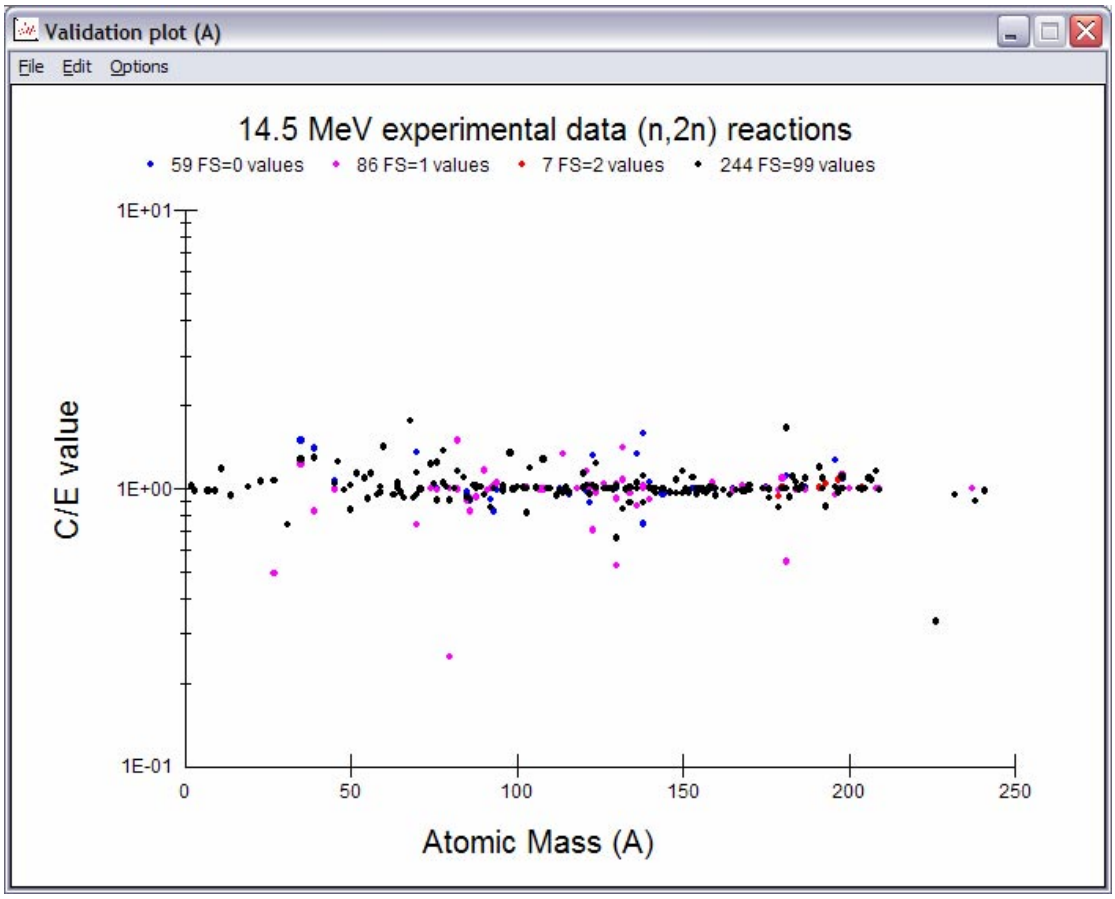


Figure 130. Validation plot (A) window.

Returning to Figure 127, the third type of plot, that of C/E or C/S as a function of the absolute value of *Q*-value can be made by selecting the x/y plot, x axis Q-value radio button. Select the other options as in the case of a histogram, then clicking the Plot button displays the Validation plot (Q) window shown in Figure 131.

Figure 131 shows the C/E data plotted as a function of the absolute value of the *Q*-value. In order to identify the various points click on one to see details presented in the status bar of the main window. It is possible to print or copy the plot to the clipboard by clicking the File|Print or Edit|Copy menu items respectively. The appearance of the graph can be altered; clicking the Options|Y axis menu item displays a submenu with five entries allowing the y axis range to be selected. In Figure 131 the option E-1 – E1 has been checked. Clicking the Options|X axis menu item displays a submenu with five entries allowing the x axis range to be selected. In Figure 131 the option 0 – 15 MeV has been checked.

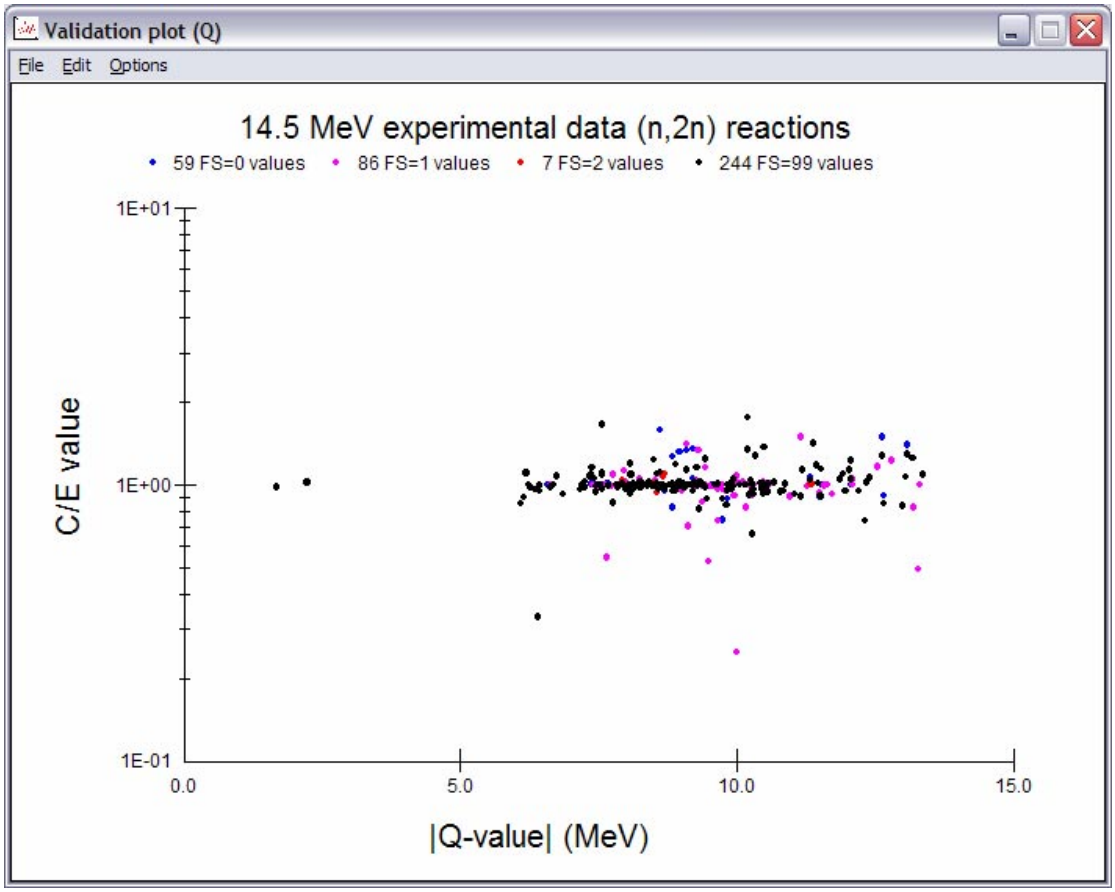


Figure 131. Validation plot (Q) window.

The discussion above on validation plots is concerned with data in the current EAF project. However, it is also useful to be able to view the validation plots for the various data sources, especially if the library covers a 'complete' set of reactions. This feature was introduced for EASY-2005. To use it a source library is selected by clicking on the Libraries|Select Source library for validation… menu item which displays the Select Source library window shown in Figure 132.

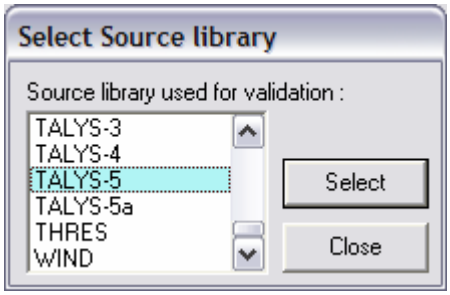


Figure 132. Select Source library window.

Selecting the required source and clicking the Select button causes the Libraries|Generate summary for <Source> library menu item to be enabled. Clicking this will generate summary data for the selected source. This is a similar process

to generating summary data for Final discussed on page 108. This can be time consumming for large source libraries.

Once the summary for the source has been generated the Libraries|Validation plots… menu item is enabled. Clicking this displys the Validation plots - <Source> window which is identical to Figure 127 except that the source name is displayed in the title bar. The discussion given above for the various graphs plotted using Final data is relevant for source data, the only differences are that the titles of the graphs show the data source being used.

It is important that all reactions have uncertainty data before the various EAF files are written. This can be tested for the threshold reactions (non-threshold reactions were checked earlier (see Figure 37) by clicking on Experimental data|Find reactions with missing threshold uncertainty data… menu item to display the Threshold reactions with missing uncert. window shown in Figure 133. Any reactions listed should be investigated further.

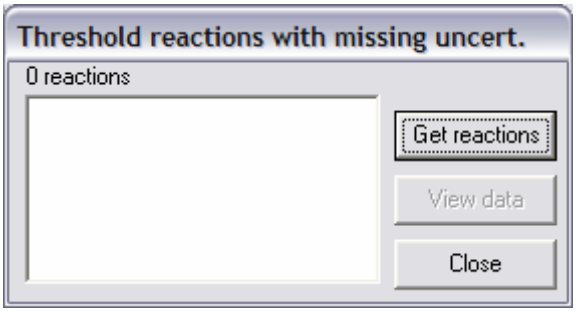


Figure 133. Threshold reactions with missing uncertainty window.

At some point prior to opening the REPORT window, and following the production of the Final database it is necessary to click on the Reaction data|Set nuclides as targets menu item. This will note which of the nuclides have cross section data and enter this into the *NucSummary* table in the Parameter database.

In SYMPAL one of the main pieces of documentation produced was the REPORT file. This was a large printed book summarising all the EAF data. It is judged that because of the highly interactive nature of SAFEPAQ-II, such a printed volume is of less interest. Rather, it is possible to view the same summary of data in a similar format as previously, but for a single reaction at a time. Clicking the Reaction data|REPORT… menu item or the twenty-ninth toolbar button displays the REPORT window shown in Figure 134. Select a target in the first list box and the reactions for that target are shown in the second list box. Clicking a reaction

shows a summary of the reaction in the data grid. Data for all final states and their sum are displayed. Values from Final, the experimental data and systematics are displayed. The modification history for each final state is shown in the History box. Data for the reaction can be printed to the default printer by clicking the Print button. Although in the future it may be implemented, there is currently no facility to print out the whole REPORT file.

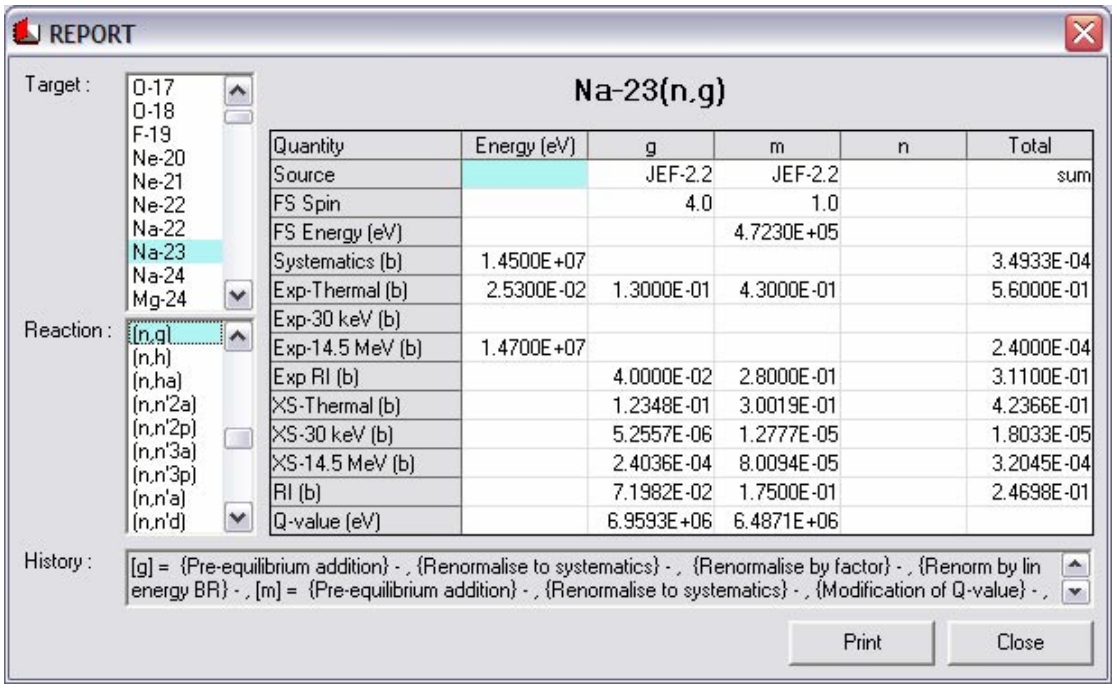

REPORT
Target :
O-17
O-18
F-19
Ne-20
Ne-21
Ne-22
Na-22
Na-23
Na-24
Mg-24
Reaction :
(n,g)
(n,h)
(n,ha)
(n,n'2a)
(n,n'2p)
(n,n'3a)
(n,n'3p)
(n,n'a)
(n,n'd)
Na-23(n,g)
Quantity | Energy (eV) | g | m | n | Total
Source | | JEF-2.2 | JEF-2.2 | | sum
FS Spin | | 4.0 | 1.0 | |
FS Energy (eV) | | | 4.7230E+05 | |
Systematics (b) | 1.4500E+07 | | | | 3.4933E-04
Exp-Thermal (b) | 2.5300E-02 | 1.3000E-01 | 4.3000E-01 | | 5.6000E-01
Exp-30 keV (b) | | | | |
Exp-14.5 MeV (b) | 1.4700E+07 | | | | 2.4000E-04
Exp RI (b) | | 4.0000E-02 | 2.8000E-01 | | 3.1100E-01
XS-Thermal (b) | | 1.2348E-01 | 3.0019E-01 | | 4.2366E-01
XS-30 keV (b) | | 5.2557E-06 | 1.2777E-05 | | 1.8033E-05
XS-14.5 MeV (b) | | 2.4036E-04 | 8.0094E-05 | | 3.2045E-04
RI (b) | | 7.1982E-02 | 1.7500E-01 | | 2.4698E-01
Q-value (eV) | | 6.9593E+06 | 6.4871E+06 | |
History :
[g] = {Pre-equilibrium addition} - , {Renormalise to systematics} - , {Renormalise by factor} - , {Renorm by lin energy BR} - , [m] = {Pre-equilibrium addition} - , {Renormalise to systematics} - , {Modification of Q-value} - ,
Print
Close

Figure 134. The REPORT window.

The tasks that now remain are to write out the Final data in EAF format. Clicking the Reaction data|Write EAF files|Write EAF_GXS files… submenu item displays the Write EAF_GXS files window shown in Figure 135. At the beginning of each EAF group file there is a 16 line header giving information about the library. The header for each group file can be created or modified in this window. Select the required Group file type radio button and then save the header by clicking the Save header button. The headers are stored in the `ascii` folder on the disk shown in the Source database disk text box in the Settings window (Figure 1). Clicking the Write all GXS files button will create the files in the folder `cross section` on the Source database disk, and Cross section data folder specified in the Settings window (Figure 1). The files have names such as `eaf_gxs_175V` indicating the group structure and weighting (this takes about 2 hours).

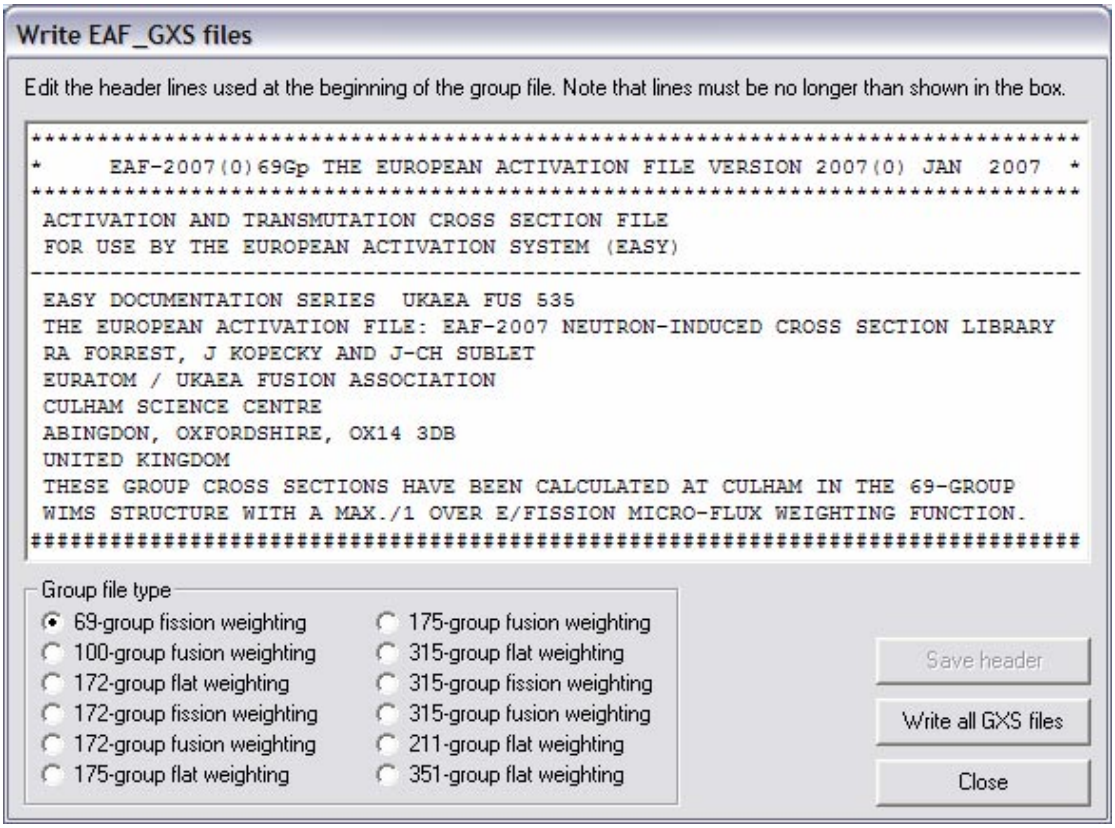

Write EAF_GXS files
Edit the header lines used at the beginning of the group file. Note that lines must be no longer than shown in the box.
****
* EAF-2007(0)69Gp THE EUROPEAN ACTIVATION FILE VERSION 2007(0) JAN 2007 *
****
ACTIVATION AND TRANSMUTATION CROSS SECTION FILE
FOR USE BY THE EUROPEAN ACTIVATION SYSTEM (EASY)
EASY DOCUMENTATION SERIES UKAEA FUS 535
THE EUROPEAN ACTIVATION FILE: EAF-2007 NEUTRON-INDUCED CROSS SECTION LIBRARY
RA FORREST, J KOPECKY AND J-CH SUBLET
EURATOM / UKAEA FUSION ASSOCIATION
CULHAM SCIENCE CENTRE
ABINGDON, OXFORDSHIRE, OX14 3DB
UNITED KINGDOM
THESE GROUP CROSS SECTIONS HAVE BEEN CALCULATED AT CULHAM IN THE 69-GROUP
WIMS STRUCTURE WITH A MAX./1 OVER E/FISSION MICRO-FLUX WEIGHTING FUNCTION.
##########
Group file type
69-group fission weighting
100-group fusion weighting
172-group flat weighting
172-group fission weighting
172-group fusion weighting
175-group flat weighting
175-group fusion weighting
315-group flat weighting
315-group fission weighting
315-group fusion weighting
211-group flat weighting
351-group flat weighting
Save header
Write all GXS files
Close

Figure 135. The Write EAF_GXS files window.

Clicking the Reaction data|Documentation menu item displays a submenu with two items. Clicking Reaction list generates a list of reactions in a readable form. A new feature introduced for EAF-2003 was the flagging of reactions that have changed since the previous EAF library. In order to do this it is necessary to have information on the previous library, this is obtained from the External database defined for Compare (see Figure 159). To check that the correct database is open the confirmation dialog shown in Figure 136 is displayed. If the External folder is correct then click the Yes button to continue, if not then Click the No button and create a new Compare database (see Figure 159). Note that the comparison means that this operation now takes longer (about 3 minutes) than in previous versions.

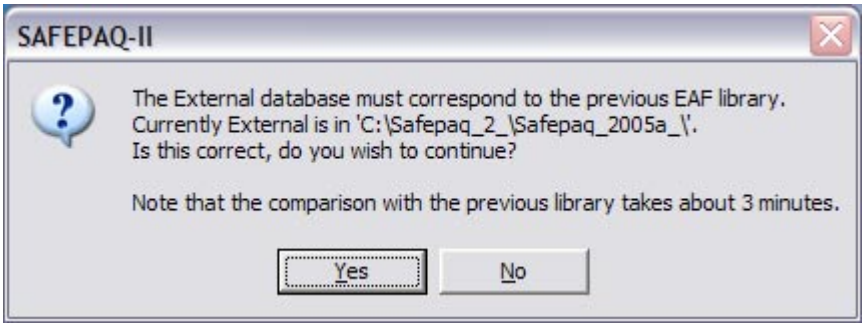

SAFEPAQ-II
The External database must correspond to the previous EAF library.
Currently External is in 'C:\Safepaq_2_\Safepaq_2005a_\'.
Is this correct, do you wish to continue?
Note that the comparison with the previous library takes about 3 minutes.
Yes
No

Figure 136. The confirmation dialog prior to writing the reaction list.

For libraries such as the EAF-2007 proton-induced one which have no previous version, there is the option of producing a simpler form of reaction list. If the database *compare.mdb* is not present in the `Safepaq_2_` folder then the dialog shown in Figure 137 is displayed. This enables the database to be generated or the reaction list to be produced with no flagging.

SAFEPAQ-II
The Compare database must be created using the previous EAF library as the External database.
Do you wish to use this to compare wih previous library?
Click 'Yes' to do this first before producing the Documentation.
Click 'No' to continue with a simple list.
Yes
No

Figure 137. The confirmation dialog if *compare.mdb* is missing.

The file (`reaction_list`) contains the source, modification history (using the Mod types shown in Table 2, the Quality score (see Table 3) and the number of data points. Clicking Source table generates a table of numbers of reactions with given MT values that are taken from the various sources (`source_table`). Both these files are located in the `Documents` folder on the disk shown in the Source database disk text box in the Settings window (Figure 1). These can be used in the production of the EAF report.

Clicking the Reaction data|Write EAF files|Write EAF_XS file submenu item creates the file `eaf_xs` in the folder `cross section` on the Source database disk, and Cross section data folder specified in the Settings window (Figure 1), this takes about 14 h. Note that in order to increase the precision of the energy and cross section values, data can be written in the ENDF scientific format. The eleven character wide field is written as ‘ `0.000000+0`’ rather than ‘ `0.0000E+00`’. Although such a format cannot be read by a standard FORTRAN format statement, there are special routines to do it. This option is set by ticking the ENDF scientific format check box in the Settings window (Figure 1).

Clicking the Reaction data|Write EAF files|Write EAF_UN file submenu item creates the file `eaf_un` in the folder `cross section` on the Source database disk, and Cross section data folder specified in the Settings window (Figure 1), this takes about 6 minutes.

In SYMPAL the reactions and their sources were available in a file `ALLReac2`. In SAFEPAQ-II this information is stored in the *ReacSummary* table in the Parameter database. To enable the

existing file to be read a reading routine is available. This is accessed from the Reaction data menu. The location of the file is the folder `ascii` on the disk shown in the Source database disk text box in the Settings window (Figure 1).

- Clicking on the Reaction data|Read ALLReac2 file menu item reads the `ALLReac2` file and enters the data into the database.

The `ALLReac2` file contains no information on the multiplicities of the reactions. These values can be entered using existing data from the Reaction data menu.

- Clicking on the Reaction data|Add multiplicities to list menu item adds the multiplicity data into the database.

These data are already present in the Parameter database, so the above methods should not be used for routine modification of the reactions. A series of windows are available to display and edit the reactions (Figure 96 - Figure 98). This is the recommended method of making changes to the reactions, as all changes will be logged.

Analysis

The data in both the Final database and in the various Data sources are so extensive that a statistical analysis can reveal underlying trends and pinpoint reactions for improvement. This approach is similar to that carried out to produce the systematics; the main difference is that for the systematics experimental data were considered while for the present analysis library data are used.

It is expected that properties such as the maximum of an excitation function and the energy at which the maximum occurs should be reasonably smooth functions of A, Z and the asymmetry parameter (s). Plotting these and also cross sections at particular energies against say A will give scatter plots that can have trend lines displayed. A full description of this Statistical Analysis of Cross Sections (SACS) is given in reference 14.

To use these tools click on the Tools|Cross section analysis… menu item to display the Cross section analysis window shown in Figure 138. Select the source of data (either Final or a Data source) in the first dropdown list and then select a reaction type from the second. For reactions such as (n,2n) which have a threshold then the Min energy textbox can be left as 0, but for say (n,p) reactions a value of 1.00E+06 eV would be appropriate (this ensures that only data above the Min energy value are considered when finding the maximum cross section.

Information on the Quality Scores are also extracted from the databases; since for split reactions the scores can be different it is necessary to specify how the score of the total cross section is calculated. There are two options: if one of the final states has a Score = 0 then the total has Score = 0 and if one of the final states is > 0 then the total has a score which is the maximum of all the final states. One of these options is selected in the Split Score group; Min: {s,0}=0 selects the first option and Max: {s,0}=s selects the second.

If information on the width of the excitation curve are required (additional time is required to find these data) then check the Include width data option which enables the Width at maximum radio button. The width refers to the width of the excitation curve at half the maximum cross section value.

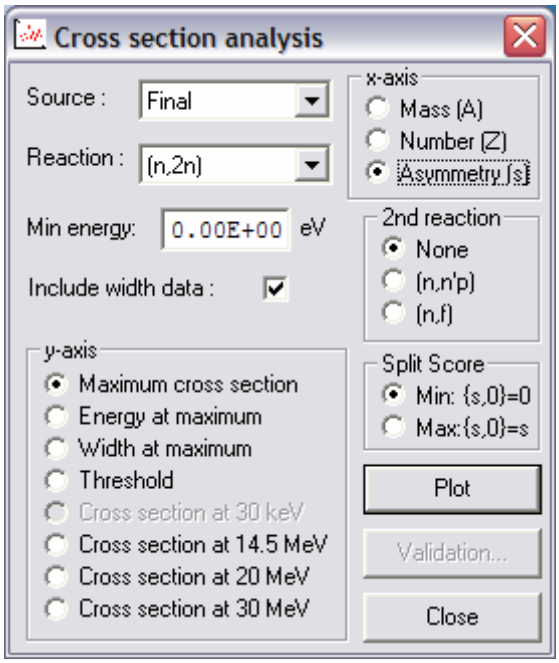


Figure 138. The Cross section analysis window.

By default the Maximum cross section radio button is selected in the y-axis group, and any of the first four options actually causes the data for all four options to be collected; this process is quite time consumming and may take several minutes. Selecting any of the remaining options causes data at the specified energy to be collected; this is typically much quicker. Note that if one of the Cross section at <energy> options is chosen then the label of the textbox changes to Delta energy, referring to the interval about the specified energy that is used to average data. This is important in cases where no data point exists at the specified energy.

By default the Mass (A) radio button in the x-axis group is selected. If the Maximum cross section radio button is selected in the y-axis group then the 2nd reaction group is

enabled and data for the selected reaction are added to the primary reaction. This is important in the case of (n,2n) where at high target mass it is appropriate to be able to consider the sum of (n,2n) and (n,f) so that the scatter can be reduced.

Clicking the Plot button will cause the data to be collected from the database, a message in the Main window status bar reminds the user that this process can be time consumming. Having collected the data then the Analysis graph window shown in Figure 139 is opened and the data displayed. Note that the number of data points are displayed in the Main window status bar. The menu bar in the Analysis graph window allows the graph to be customised as required. Clicking the Options|Axis scale… menu item displays the Axis scale window (Figure 84) where the axis ranges on the x- and y-axes can be changed. Clicking the Options|Distinguish Even/Odd menu item will show the various Even and Odd combinations of *Z* and *N* for the targets in various colours and affords another method of spotting trends. Clicking the Options|Distinguish Importance menu item will indicate if the reaction is included in the list of important reactions given in reference 15 by the use of two colours. Clicking the Options|Distinguish Scores menu item will indicate whether the reactions have Quality Score > or = 0 by the use of two colours. These three menu items act as toggles and the ticks indicates which option is selected.

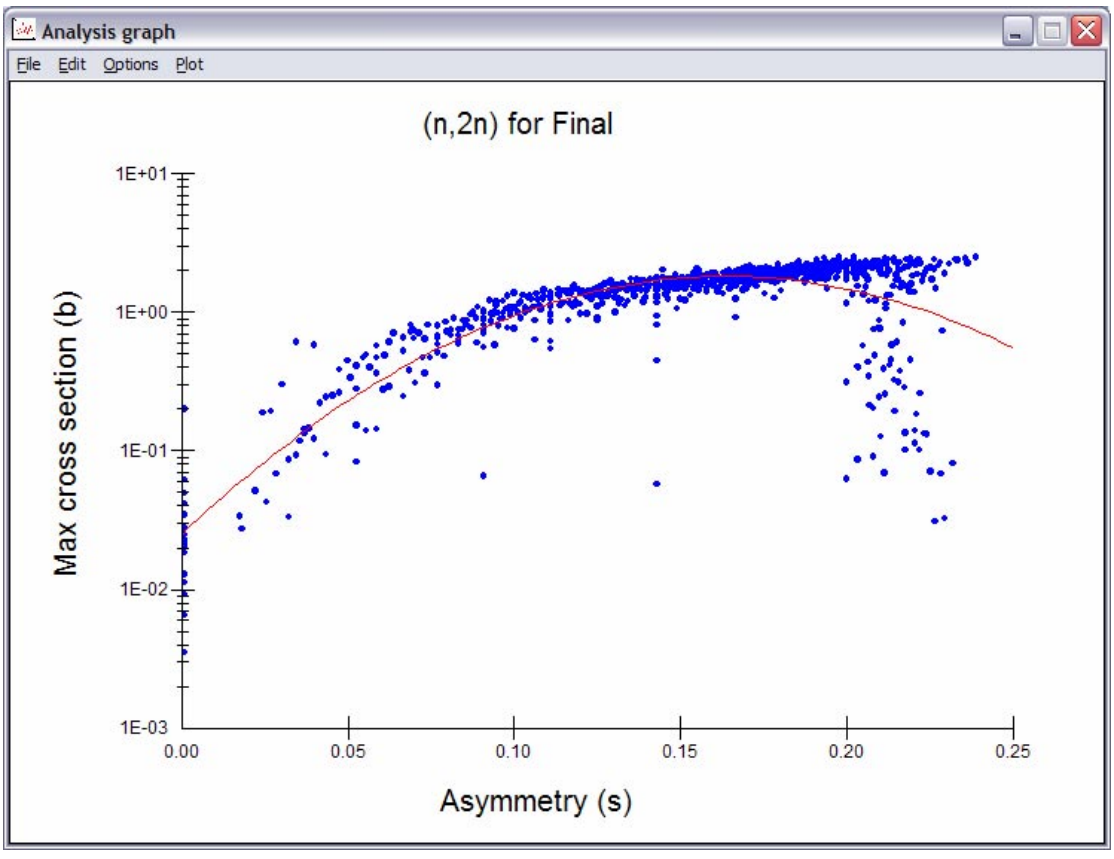


Figure 139. The Analysis graph window.

If a point is clicked with the right mouse button then it can be excluded from the display. If the Options|Allow symbol change menu item is checked then it is possible to show particular points as a red triangle (instead of the usual blue circle) so allowing particular points to be identified when the graph is copied to an external document. This can be done by clicking the point with the middle mouse button or by clicking the Options|Change symbol for nuclide… menu item which displays a small dialog shown in Figure 140 which enables a target nuclide to be entered.

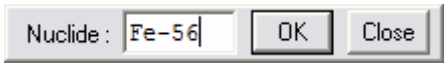


Figure 140. The Change symbol for nuclide window.

Clicking the OK button will change the symbol and clicking the Close button will close the window. By default the data are plotted in colour as shown in Figure 139, by clearing the tick on the Options|Colour menu item, data are shown in black symbols which may be more appropiate for a black and white printer. If the one of the Options|Distinguish <something> menu items is ticked then the position of the legend on the graph can be altered by selecting one of the options (Top or Bottom) on the Options|Legend submenu.

The graph is 'Hot', clicking with the mouse on one of the data points shows the identity and details of the reaction. A trend line can be added to the graph (as shown in Figure 139) by means of a least squares line of best-fit. Clicking the Options|Trend line menu item displays or clears the line. Two types of fit can be used. Checking the Options|Curve type|Power menu item causes the functional form shown in equation 4 to be used for the trend curve.

$$\sigma = 10^{\alpha+\beta x+\gamma x^2+\delta x^3} \qquad (4)$$

Checking the Options|Curve type|Logarithmic menu item causes the functional form shown in equation 5 to be used for the trend curve. In equations 4 and 5 x can be A, Z or s.

$$\sigma = Ax^B \qquad (5)$$

The order (1, 2 or 3) of the polynomial used for the fitting in equation 4 can be chosen from the Options|Curve order submenu. If the curve order is 1 then γ and δ are 0, if 2 then δ is 0, and if 3 then all of α, β, γ, δ are non-zero. Note that if a Logarithmic curve is chosen then the Options|Curve order menu item is disabled.

The trend line can be displayed as a thick or thin line depending on whether the Options|Draw lines thick menu item is checked or cleared. The form of the equation can be displayed in the Main window status bar by clicking the Options|Display equation menu item. A trend line can be stored by clicking the Options|Store trend menu item, this trend can then be used in the Validation plots window (Figure 127).

At the present time details for only a subset of the reactions and trend curve options can be stored. $\sigma_{max}(A)$ and $\sigma_{max}(s)$ trends for the reaction types: (n,2n), (n,3n), (n,4n), (n,p), (n,d), (n,t), (n,h) and (n,α) can be stored. Trends for the Power and Logarithmic curves can be stored, but in the case of a Power curve only for the Curve order 2 option (α, β, γ are non-zero in equation 4).

It is possible to exclude various points. The Options|Plotted points submenu shows a series of options. By default Options|Plotted points|All is checked and all the points are shown. If Options|Plotted points|Not excluded is checked then any of the options listed below that are checked are not plotted. Checking Options|Plotted points|Exclude actinides ensures that all reactions where the target has $Z > 85$ are excluded. Checking Options|Plotted points|Exclude A < 20 ensures that all reactions where the target has $A < 20$ are excluded. Checking Options|Plotted points|Exclude A < 40 ensures that all reactions where the target has $A < 40$ are excluded. Checking Options|Plotted points|Exclude Scores = 0 ensures that all reactions that have a Quality Score of 0 are excluded. Checking Options|Plotted points|Exclude Scores > 0 ensures that all reactions that have a Quality Score > 0 are excluded. Checking Options|Plotted points|Exclude Unimportant ensures that all reactions that are not in the list of important reactions are excluded. Checking Options|Plotted points|Exclude Important ensures that all reactions that are in the list of important reactions are excluded.

It is possible to return to the cases where all points are plotted by clicking the Options|Plotted points|Reset, none excluded menu item, and all points can be plotted with the standard symbol by clicking the Options|Plotted points|Reset, standard symbols menu item. When the graph is redrawn the actual number of points plotted is shown in the Main window status bar.

Once a trend line is shown then the Options|Reaction details… menu item is enabled. Clicking this displays the Reaction details window shown in Figure 141. The type of reaction and the data source are shown on the window title bar. By default all the reactions are listed, sorted by the ZA value of

the target. By selecting one of the > Factor <n> radio buttons only a subset of the reactions significantly far from the trend line are listed. Note that it is possible to sort the data by any of the column values, clicking on the appropriate Sort button will reorder the data, a single click causes the button to display Sort V (descending) a second click shows Sort A (ascending). The data can be returned to the default order by clicking the Reset button over the first column.

If points have been excluded in the plot then they can also be excluded from the Reaction details window. Clicking the As graph option in the Exclude group and then clicking the Get reactions button shows the reduced list. So long as the All reactions option is selected then two Confidence intervals are displayed. In Figure 141 these show that 68% of the points are within a factor of 1.41 of the trend line and 95.5% are within a factor 3.76.

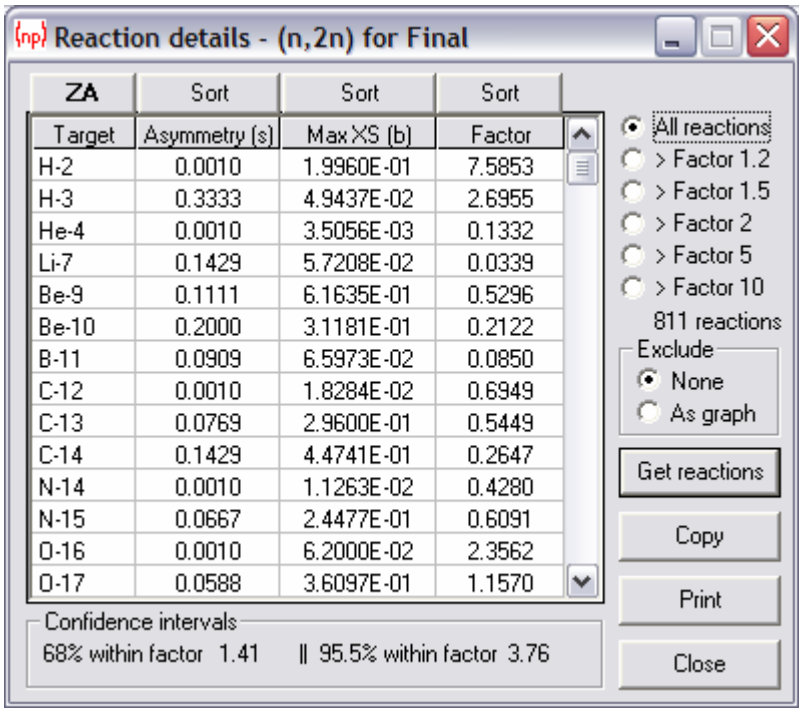


Figure 141. The Reaction details window.

The selected items in the grid can be copied to the clipboard by clicking the Copy button. The entire listing can be printed to the default printer by clicking the Print button. The window can be closed by clicking the Close button.

Returning to the Analysis graph window (Figure 139); clicking the Edit|Copy menu item places the graph on the clipboard. Clicking the Edit|Copy coefficients menu item copies the Trend line coefficients onto the clipboard using 4 decimal places. This gives a higher accuracy than in the Main

window status bar and is useful if the equation is to be used for other studies.

In the earlier discussion of validation plots, the option of producing C/T plots was mentioned in the Validation plots window (Figure 127). These can only be produced by opening an extended version of the window. Clicking the Validation… button displays the extended version of the Validation plots window (Figure 142). It will be noted that the C/T type option is selected by default and that two additional sets of options are available: the variable on the C/T axis (either A or s) and the Trend type (Log or Power). Note also that it is not possible to change the Graph type, the Energy or the Final state. The choice of Reaction, C/T axis and Trend type are determined by the type of Analysis chosen in the Cross section analysis and Analysis graph windows. Clicking the Plot button displays the Validation plot window shown in Figure 143. The title shows the various options chosen.

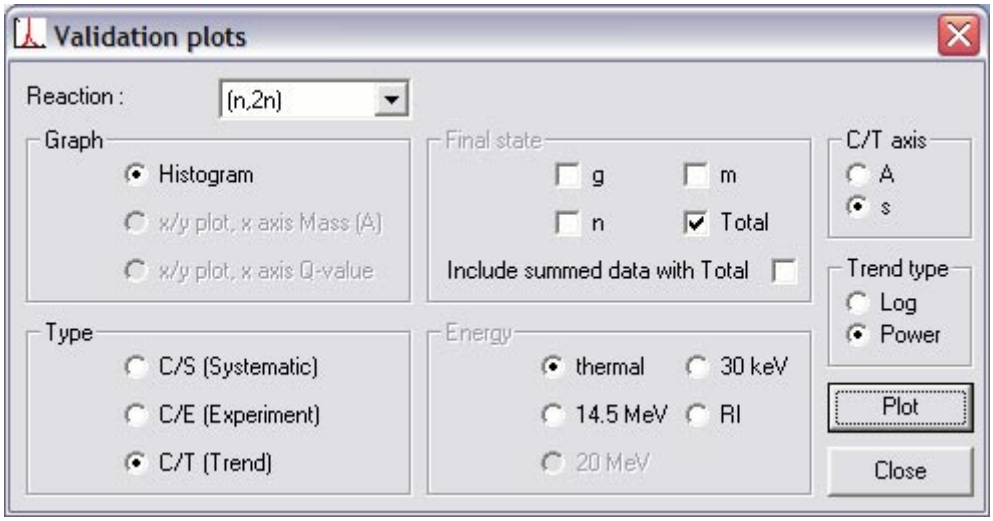


Figure 142. Validation plots (extended) window.

The graph can be printed to the default printer by clicking the File|Print menu item, and the window can be closed by clicking the File|Close menu item. Note that if the Cross section analysis window is closed while the other two are still open then they are automatically closed as well. The Plot menu item allows the graph to be redrawn.

Changing the various options in the Cross section analysis window and then clicking the Plot button will typically quickly refresh both the Analysis graph and Reaction details windows if they are open. However, if a different reaction source or type is chosen then a lengthy collection process will be needed before the graph is redrawn.

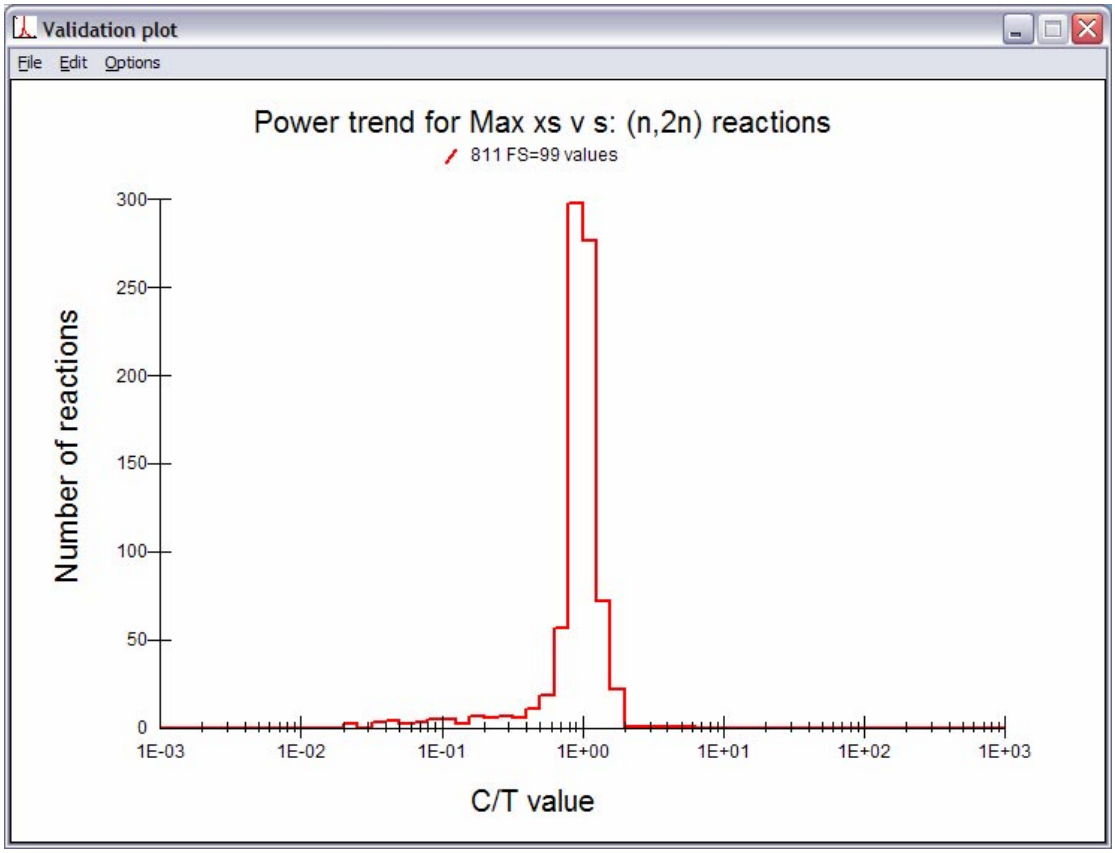


Figure 143. Validation plot (C/T) window.

Miscellaneous tools

It is often useful to know the *Q*-value for a reaction. Clicking on the Tools|Calculate Q-value… menu item displays the Calculate Q-value window shown in Figure 144. Enter the target in the text box and select the reaction from the dropdown list. Clicking the Calculate button displays the *Q*-value and the threshold. The window is closed by clicking the Close button.

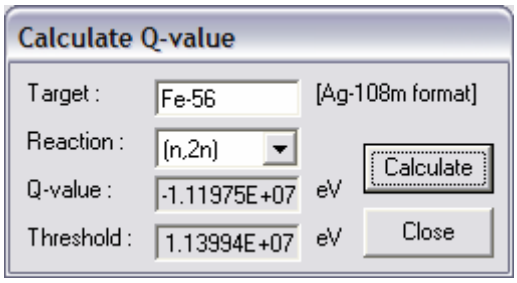


Figure 144. The Calculate Q-value window.

Systematic formulae are used for many purposes in SAFEPAQ-II. Details of these are available in the EASY documentation [10]. The values used for the various reactions and energies can be seen by clicking on the Tools|Calculate systematics… menu item, this displays the Calculate systematics window shown in Figure 145. Enter the target in the text box and select

the reaction from the dropdown list. Clicking the Calculate button displays the available systematics values. Depending on the reaction type, systematics at one, two or three energies are displayed. By default the standard sytematics formulae are used, but if the Experimental data|Systematics|Alternate submenu item is checked then the alternate set of formulae are used in the calculations. The window is closed by clicking the Close button.

If the reaction chosen is (n,n′) then the window has additional options as shown in Figure 146. Only the 3 MeV value is shown (instead of the standard 30 keV value), and the final state of the daughter must be chosen in the Final state group by selecting one of the g, m or n radio buttons.

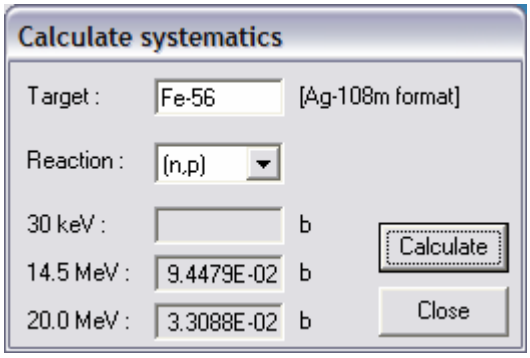


Figure 145. The Calculate systematics window.

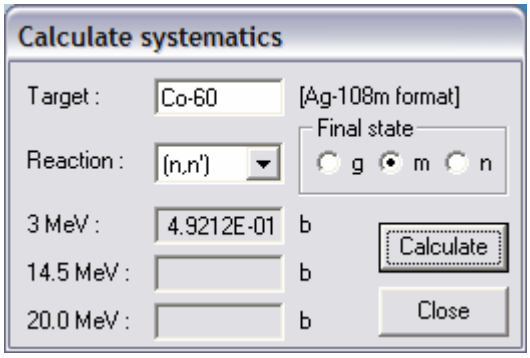


Figure 146. The Calculate systematics window for (n,n′) reaction.

While working with SAFEPAQ-II it is often useful to be able to find the atomic number (Z) for particular elements. This can be found by clicking on the Tools|View elements… menu item that displays the Elements window shown in Figure 147. This shows Z and the chemical symbol for each element. The name corresponding to the symbol can be seen by selecting an element and the name is shown in a ToolTip. The window is closed by clicking the Close button.

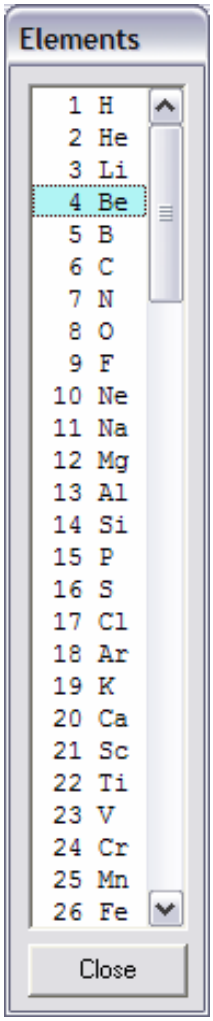


Figure 147. The Elements window.

The type of reaction is shown in ENDF files by means of the MT value. A list of MT numbers can be seen by clicking on the Tools|View MT numbers… menu item that displays the MT numbers window shown in Figure 148. This shows MT and the conventional symbol for each reaction. The standard ENDF MT numbers appear above the dividing line, those below are non-standard ones defines in EASY for extended energy libraries. The window is closed by clicking the Close button.

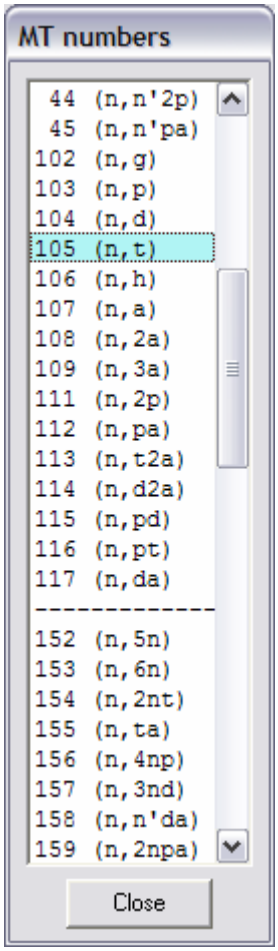


Figure 148. The MT numbers window.

The Mod types of the various modifications are shown in Table 2. A list of the Mod types can be seen by clicking on the Tools|View Modification types… menu item that displays the Modification types window shown in Figure 149. This shows the Mod types and the corresponding action for each modification. The window is closed by clicking the Close button.

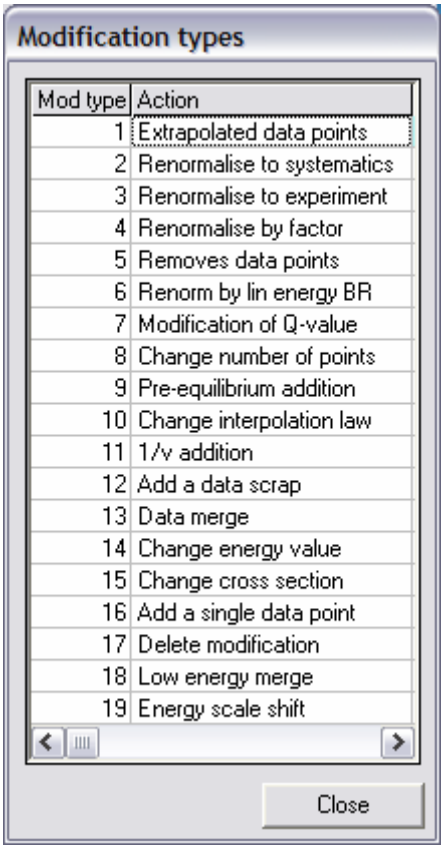


Figure 149. The Modification types window.

If SAFEPAQ-II crashes during data entry it is possible that the Final database can be left in a damaged state. Typically there is an entry for a reaction in the Parameter database, but this is missing in Final. This means that it is not possible just to add the reaction (using Figure 97) and the reaction is not present when using Single reaction processing (Figure 119). To correct this situation click on the Tools|Repair Final… menu item to display the Repair Final window shown in Figure 150.

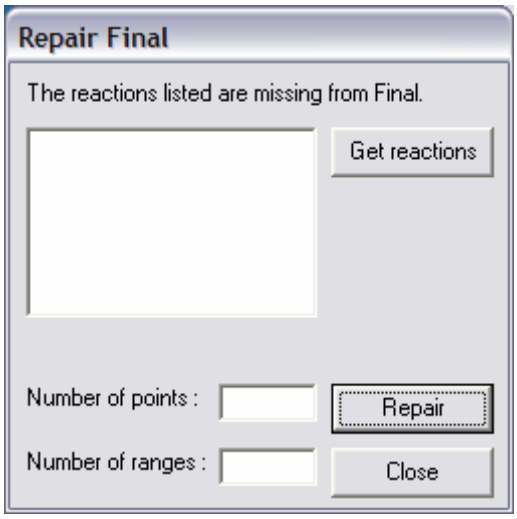


Figure 150. The Repair Final window.

Clicking the Get reactions button displays any reactions missing from Final but present in Parameter in the list box. Clicking on a reaction displays a message describing which tables the reaction is missing from and where possible showing the number of data points and interpolation ranges in the text boxes. Clicking the Repair button will add the reaction details back into the Final database tables using data from Master. There is now an entry for the reaction, but the actual data may not be correct, a warning dialog box informs the user that the data should be corrected using the Single reaction processing window (Figure 119). The window is closed by clicking the Close button.

If SAFEPAQ-II crashes it is possible that one of the Access databases can be damaged. If this happens then during use of SAFEPAQ-II an error message will be displayed stating that the file is not in database format when the application tries to open the damaged database. It is usually possible to repair such damage and return the database to a usable state. To do this click on the Tools|Repair databases… menu item to display the Repair databases window shown in Figure 151. Select the database to be repaired and click the Repair button.

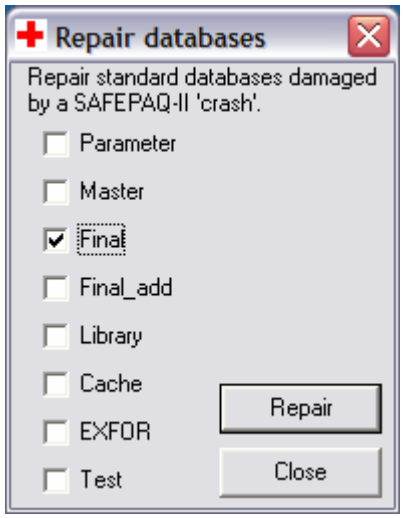


Figure 151. The Repair databases window.

As SAFEPAQ-II is developed new features are added. In most cases this means that the SQL queries in the various databases are either amended or new ones added. It follows that if an old database is used with the current version of SAFEPAQ-II then it can crash because the code calls non-existent queries. This can be corrected by importing the new or modified queries into the old database. There can be many such changes, so this process is automated by clicking on the Tools|Update databases… menu item to display the Update databases window shown in Figure 152.

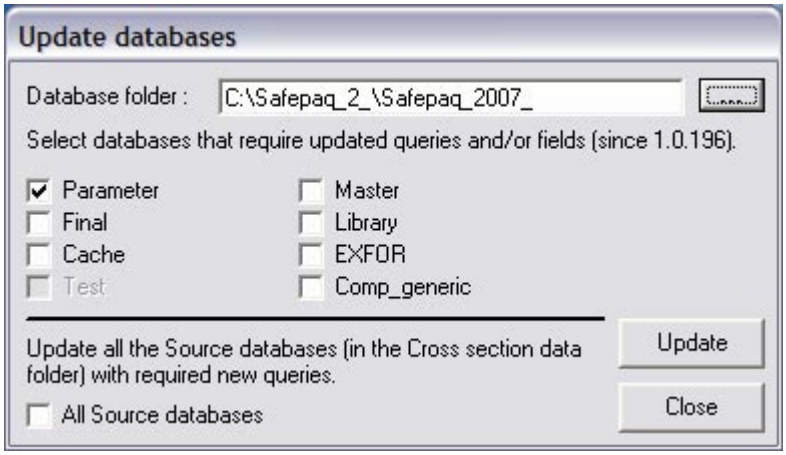


Figure 152. The Update databases window.

Click the browse button (…) to display the Open dialog and select one of the databases in the folder containing the SAFEPAQ-II databases needing to be updated. The folder name is displayed in the text box. Depending on the SAFEPAQ-II version only some of the databases need to be updated, these are shown with the check boxes enabled. Select the ones required (usually select all possible) and click the Update button. This adds all the new queries to the selected databases.

Sometimes the various source databases need to be similarly updated. This can be done by ticking the All Source databases check box in the lower part of the window. Note that even if only the source databases need to be updated it is still necessary to select a database folder (ensure that none of the database check boxes are ticked). The window is closed by clicking the Close button.

SAFEPAQ-II is continually improved with new features and errors in the coding corrected. This is reflected in the Version number displayed in the About SAFEPAQ-II window (Figure 8). Keeping track of bugs and requests for new features is important and a feature to do this has been added for EAF-2007. In addition other parts of EASY also need to have bugs and new features recorded. This feature is only available for the developer of the code system (R.A. Forrest). Another Access database (*Helpdesk_.mdb*) is held in the `Safepaq_2_` folder. Clicking the Tools|Helpdesk menu item displays a submenu containing the items New, Edit and List entries…. Clicking the New|Person… menu item displays the New person window shown in Figure 153. Select a Title from the dropdown list and enter details in the text boxes. Clicking the Save button stores the information in the *Helpdesk_.mdb* database (following a confirmation dialog) and clicking the Close button closes the window.

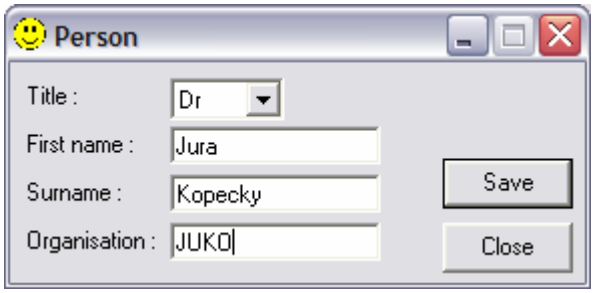


Figure 153. The New person window.

Clicking the New|Entry… menu item displays the New entry window shown in Figure 154. Select one of the already defined people from the Person dropdown list. The type of entry is selected from the Type dropdown list (FISPACT, SAFEPAQ-II, User Interface, EAF and Documentation are the options). The source of the entry is selected from the Source dropdown list (Phone, e-mail, Discussion, Document, Idea are the options) and a reference to it given in the Reference textbox. A description of the entry is added to the Description textbox and today's date is automatically entered in the Date created textbox. Typically the Response and Date finished textboxes are left blank. Clicking the Save button stores the information in the *Helpdesk_.mdb* database (following a confirmation dialog) and clicking the Close button closes the window.

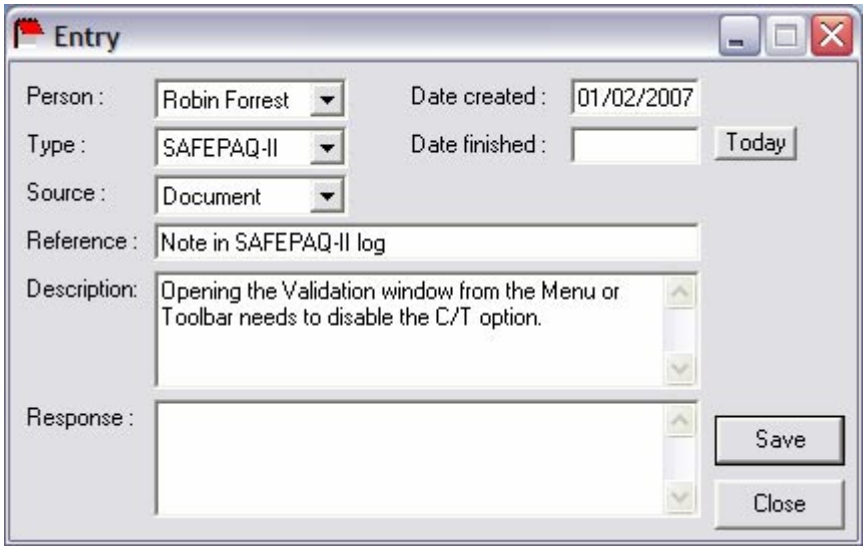


Figure 154. The New entry window.

The details of a person already defined can be edited by clicking the Edit|Person… menu item which displays the Edit person window shown in Figure 155. Enter a Surname and click the Get person button to display the details of the person. If more than one person with the same name has been defined then the > and < buttons allow details for each one to be displayed. The Title, First name and Organisation can be changed if required and the changes stored in the database by

clicking the Save button. Clicking the Close button closes the window.

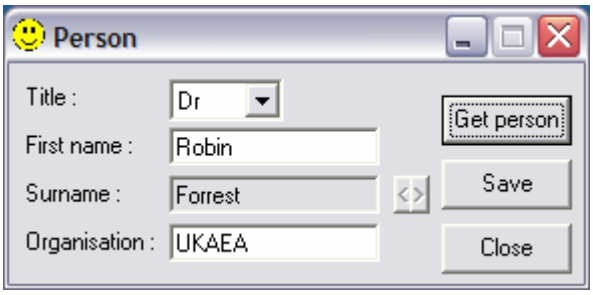


Figure 155. The Edit person window.

A list of the available enties can be found by clicking the Tools|Helpdesk|List entries… menu item which displays the List entries window shown in Figure 156. Select an entry from the List by dropdown list (Surname, Organisation, Type, Source, Before date, Unfinished and Completed are options). In the first five cases a criterion must be entered in the Criteria combo box (if a suitable criterion is available in the dropdown list then it can be selected). Clicking the List button will display the selected entries. The list can be printed by clicking the Print button. Select an entry in the list and click on the Edit button to display the Edit entry widow which is identical to Figure 154. It is now possible to enter information in the Response and Date finished textboxes. If the entry was completed today then today's date can be entered by clicking the Today button. The changes can be stored in the database by clicking the Save button. Clicking the Close button closes the window.

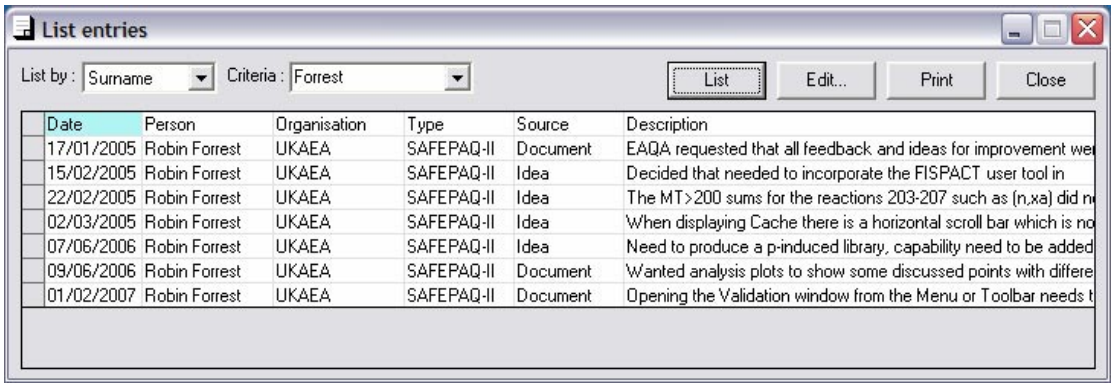

List entries
List by : Surname
Criteria : Forrest
List
Edit...
Print
Close
Date Person Organisation Type Source Description
17/01/2005 Robin Forrest UKAEA SAFEPAQ-II Document EAQA requested that all feedback and ideas for improvement wer
15/02/2005 Robin Forrest UKAEA SAFEPAQ-II Idea Decided that needed to incorporate the FISPACT user tool in
22/02/2005 Robin Forrest UKAEA SAFEPAQ-II Idea The MT>200 sums for the reactions 203-207 such as (n,xa) did n
02/03/2005 Robin Forrest UKAEA SAFEPAQ-II Idea When displaying Cache there is a horizontal scroll bar which is no
07/06/2006 Robin Forrest UKAEA SAFEPAQ-II Idea Need to produce a p-induced library, capability need to be added
09/06/2006 Robin Forrest UKAEA SAFEPAQ-II Document Wanted analysis plots to show some discussed points with differe
01/02/2007 Robin Forrest UKAEA SAFEPAQ-II Document Opening the Validation window from the Menu or Toolbar needs t

Figure 156. The List entries window.

It is important to keep track of the users of EASY so that, for instance, they can be notified of new versions. PC users also require a serial number and password. A database of users is only available to the developer of the code system (R.A. Forrest) in another Access database (*Users_.mdb*) held in the `Safepaq_2_` folder. Clicking the Tools|Users menu item displays a submenu containing the items New user… and Edit user…. Clicking the New user… menu item displays the New

user window shown in Figure 157. Enter details of the user, and whether the version of EASY is an internal one or a commercial sale. Select the EASY versions and platform and then click the Add button to store the information in the database (following a confirmation dialog). Clicking the Close button closes the window.

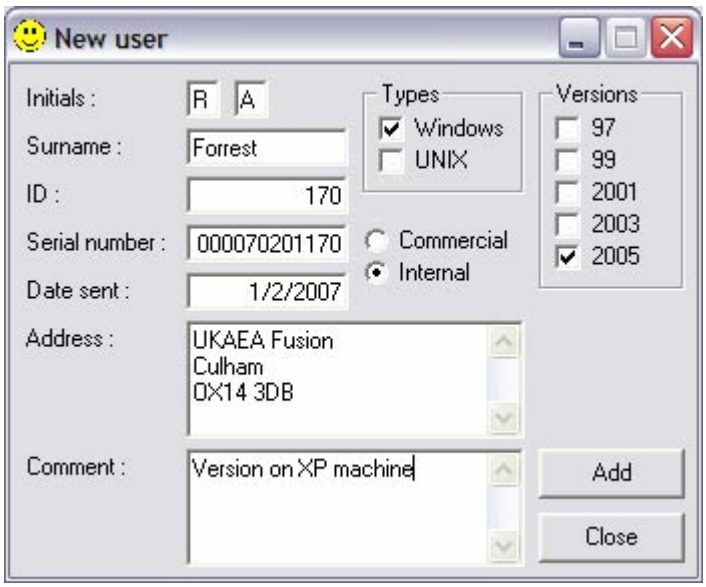


Figure 157. The New user window.

Clicking the Tools|Edit user… menu item displays the Edit user window shown in Figure 158. A user can be selected from the Surname dropdown list which displays their details. Certain details such as Initials, ID and Serial number cannot be changed. Click the Save button to store the information in the database (following a confirmation dialog). Clicking the Close button closes the window.

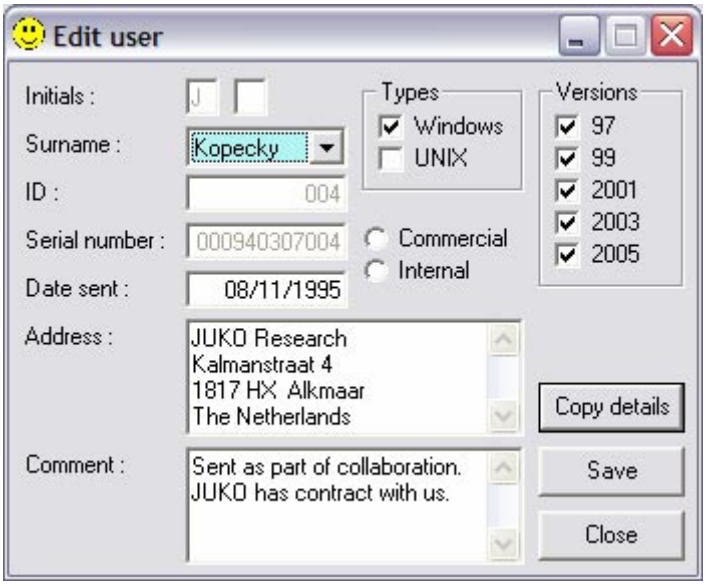


Figure 158. The Edit user window.

Clicking the Copy details button copies user information (Name, Serial number and Password) onto the clipboard. These details are required when the EASY User Interface software is installed.

Updating databases

A major advantage of developing SAFEPAQ-II as a Windows application is that it enables several users to participate in producing EAF libraries. These users are in separate countries and so there is the question of how their contributions can be integrated to form the final library. It is possible to design the Access databases so that there is a single 'Design Master' and several 'Replica' databases. When changes are made to the Replicas, these can be reconciled in the Design Master by a process of 'synchronization' which ensures that all copies are identical. Such a process is automatic, and there is no possibility of choosing if all changes should be implemented. Also there are certain technical differences in the structure of the databases in a 'Replica set', the most important being that auto-number fields are added randomly rather than in numerical order. It therefore seemed better to carry out the updating in a more manual fashion.

All information on a particular library version is held in the Parameter database. In addition choices about experimental data to be used for visualisation are held in the EXFOR database. It is only necessary therefore to have copies of these two databases (which are relatively small compared to Final) to compare with the original (which is held at Culham). A series of queries using tables from the original (termed the Internal) and the copy (termed the External) databases have been developed. These are held in a new database *compare.mdb*. Actually, there is a database *comp_generic.mdb* that contains all the queries but no tables. When it is necessary to compare the Internal and External databases a new version of Compare is produced which contains links to tables in the Internal and External databases. This is done by clicking on the Tools|Create Compare database… menu item which displays the Create Compare database window shown in Figure 159. Note that the current External folder is shown, and so this window can be used if the location of the External folder is required for other purposes.

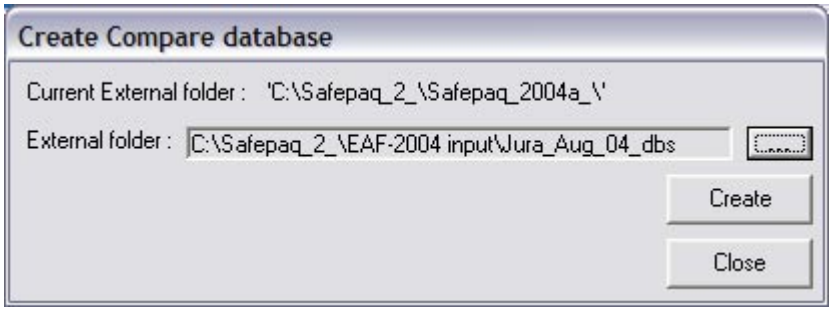


Figure 159. The Create Compare database window.

Clicking the browse button (…) displays the standard Open dialog where the folder containing the External databases can be selected. Clicking the Create button copies *comp_generic.mdb* to *compare.mdb* and links all the required tables. If Compare already exists then a confirmation dialog is displayed. Once the Compare database has been created (in the current SAFEPAQ folder), a set of menu items on the Tools menu become enabled. These enable a series of comparisons to be carried out.

Clicking the Tools|Compare|Reaction sources… submenu item displays the Compare reaction sources window shown in Figure 160. This shows reactions where the data source is different between the Internal and External databases. The contents of the grid can be copied or printed by clicking on the Copy or Print buttons respectively.

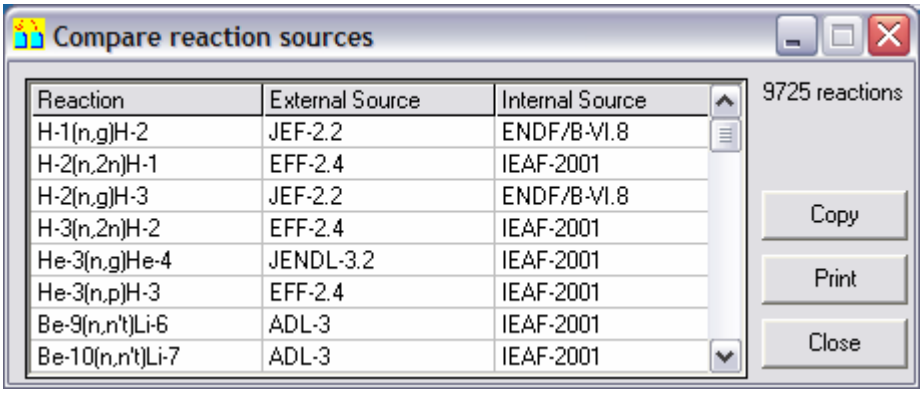


Figure 160. The Compare reaction sources window.

Clicking the Tools|Compare|References… submenu item displays the Compare references window shown in Figure 161. This shows new references in External that are not in Internal. The contents of the grid can be copied or printed by clicking on the Copy or Print buttons respectively.

Clicking the Tools|Compare|Experimental data flags… submenu item displays the Compare experimental data flags window shown in Figure 162. This shows data sets where the flags (these show if the experimental data are used for

branching, renormalisation or validation) are different between Internal and External for matching data sets. In the grid headings 'I' refers to the internal and 'E' to the External databases. The contents of the grid can be copied or printed by clicking on the Copy or Print buttons respectively.

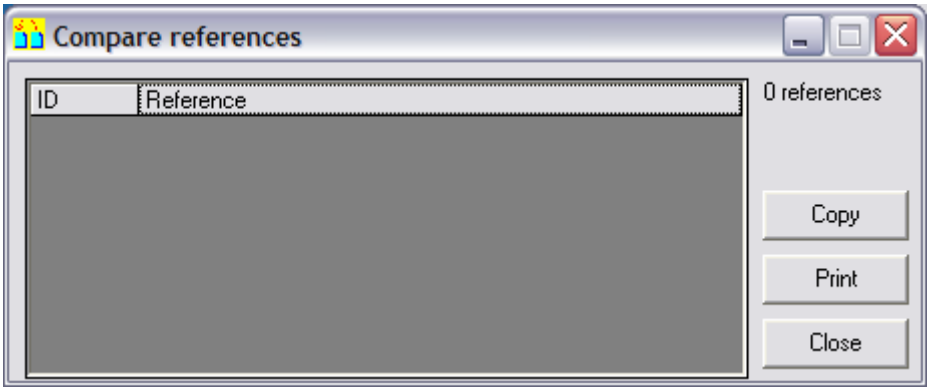


Figure 161. The Compare references window.

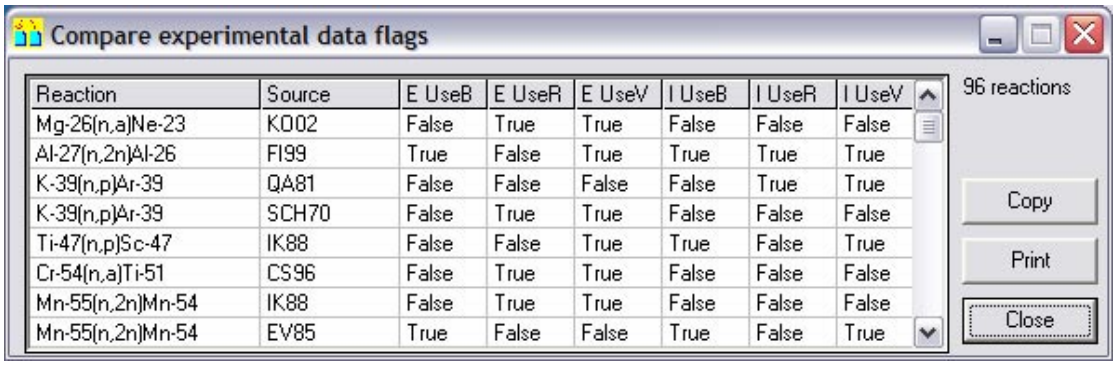

Compare experimental data flags
Reaction Source E UseB E UseR E UseV I UseB I UseR I UseV
Mg-26(n,a)Ne-23 KO02 False True True False False False
Al-27(n,2n)Al-26 FI99 True False True True True True
K-39(n,p)Ar-39 QA81 False False False False True True
K-39(n,p)Ar-39 SCH70 False True True False False False
Ti-47(n,p)Sc-47 IK88 False False True True False True
Cr-54(n,a)Ti-51 CS96 False True True False False False
Mn-55(n,2n)Mn-54 IK88 False True True False False False
Mn-55(n,2n)Mn-54 EV85 True False False True False True
96 reactions
Copy
Print
Close

Figure 162. The Compare experimental data flags window.

Clicking the Tools|Compare|New experimental data… sub-menu item displays the Compare new experimental data window shown in Figure 163. This shows reactions where there are new data sets in External that are not present in Internal and the values that are in External. The contents of the grid can be copied or printed by clicking on the Copy or Print buttons respectively.

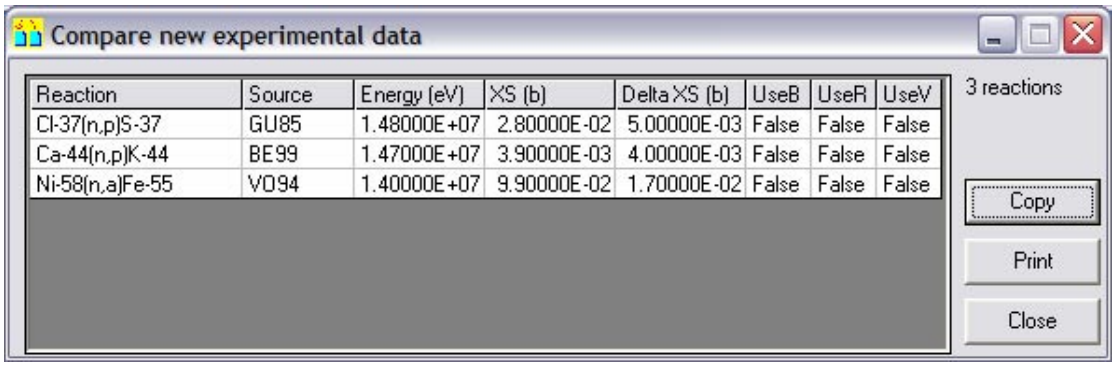

Compare new experimental data
Reaction Source Energy (eV) XS (b) Delta XS (b) UseB UseR UseV
Cl-37(n,p)S-37 GU85 1.48000E+07 2.80000E-02 5.00000E-03 False False False
Ca-44(n,p)K-44 BE99 1.47000E+07 3.90000E-03 4.00000E-03 False False False
Ni-58(n,a)Fe-55 VO94 1.40000E+07 9.90000E-02 1.70000E-02 False False False
3 reactions
Copy
Print
Close

Figure 163. The Compare new experimental data window.

Clicking the Tools|Compare|Systematics data flags… sub-menu item displays the Compare systematics data flags window shown in Figure 164. This shows reactions where there are differences in the usage flags for systematics. The values of the UseR and UseB fields in the External and Internal databases are shown. The contents of the grid can be copied or printed by clicking on the Copy or Print buttons respectively.

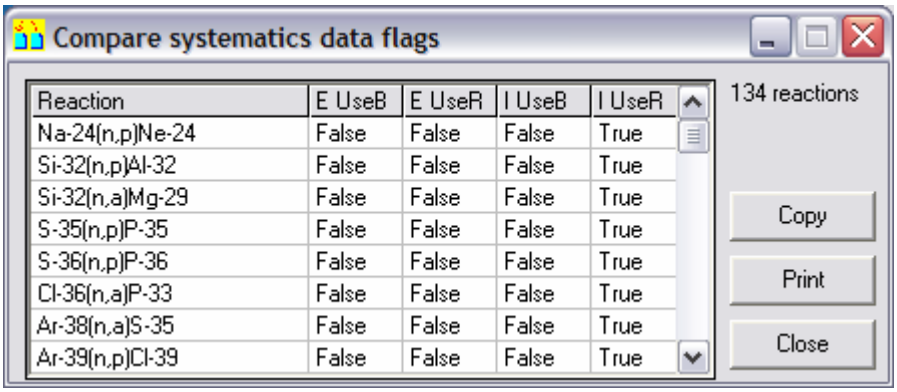


Figure 164. The Compare systematics data flags window.

Clicking the Tools|Compare|New systematics flags… sub-menu item displays the Compare new systematics flags window shown in Figure 165. This shows reactions where there are new systematics data flags in the External database. The values of the UseR and UseB fields in the External database are shown. The contents of the grid can be copied or printed by clicking on the Copy or Print buttons respectively.

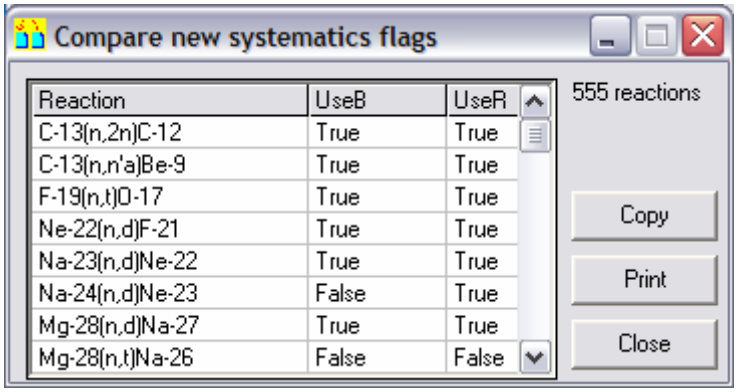


Figure 165. The Compare new systematics flags window.

Clicking the Tools|Compare|Removed systematics flags… submenu item displays the Compare removed systematics flags window shown in Figure 166. This shows reactions where systematics data flags for a reaction have been removed in the External database. The values of the UseR and UseB fields in the Internal database are shown. The contents of the grid can be copied or printed by clicking on the Copy or Print buttons respectively.

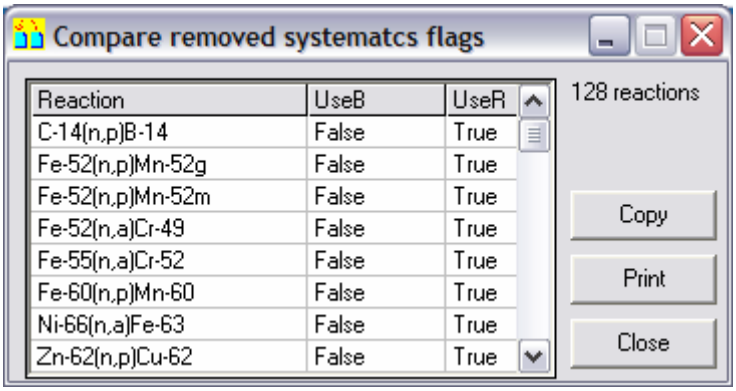


Figure 166. The Compare removed systematics flags window.

Clicking the Tools|Compare|Integral data… submenu item displays the Compare integral data window shown in Figure 167. This shows reactions where there are differences in the integral data between the Internal and External databases. The contents of the grid can be copied or printed by clicking on the Copy or Print buttons respectively.

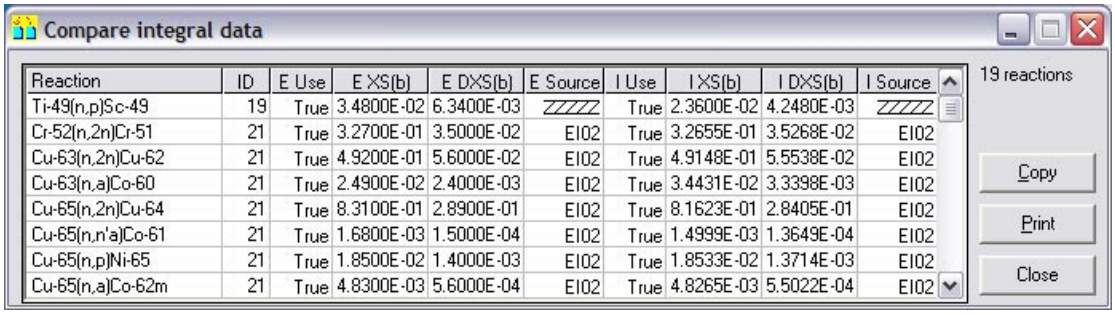


Figure 167. The Compare integral data window.

Clicking the Tools|Compare|New Integral data… submenu item displays the Compare new integral data window shown in Figure 168. This shows reactions where there are new integral data in the External database. The values of the integral data in the External database are shown. The contents of the grid can be copied or printed by clicking on the Copy or Print buttons respectively.

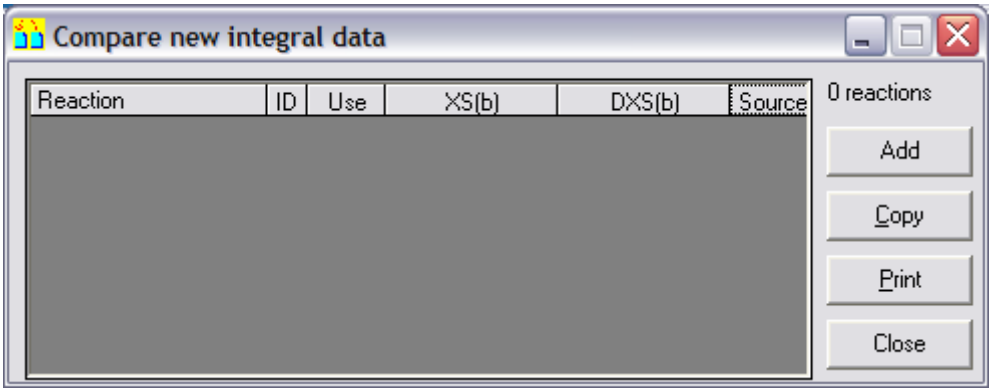


Figure 168. The Compare new integral data window.

Clicking the Tools|Compare|Number of pre-modifications… submenu item displays the Compare number of pre-modifications window shown in Figure 169. This shows reactions where there are differences in the number of pre-modifications in the External and Internal databases. To discover what the External pre-modifications are click on the reaction to display a ToolTip containing all the details. If there is more that one pre-modification then pressing the '>' or '<' keys will display the next or previous pre-modification details. If changes are made to the pre-modifications while the window is open then the list can be refreshed by clicking the Refresh button. The contents of the grid can be copied or printed by clicking on the Copy or Print buttons respectively.

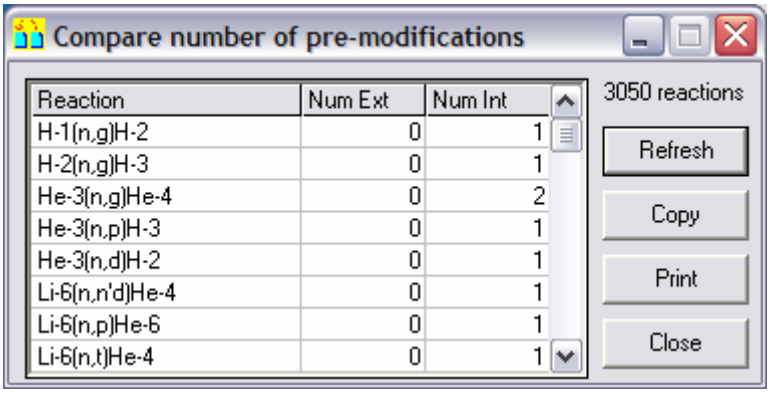


Figure 169. The Compare number of pre-modifications window.

Clicking the Tools|Compare|Number of modifications… submenu item displays the Compare number of modifications window shown in Figure 170. This shows reactions where there are differences in the number of modifications in the External and Internal databases. To discover what the External modifications are click on the reaction to display a ToolTip containing all the details. If there is more that one modification then pressing the '>' or '<' keys will display the next or previous modification details. The contents of the grid can be copied or printed by clicking on the Copy or Print buttons respectively.

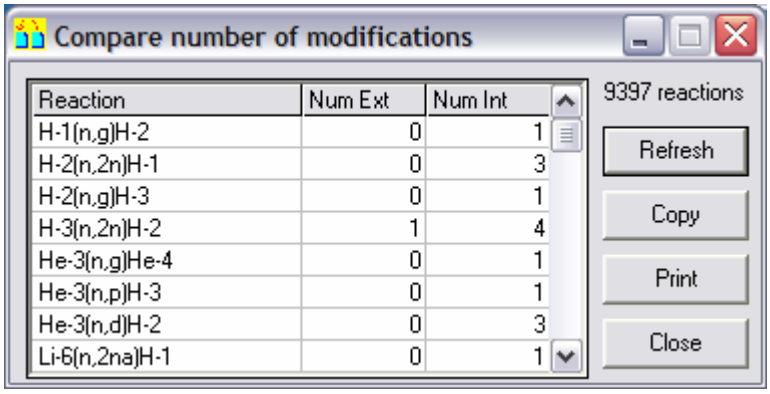


Figure 170. The Compare number of modifications window.

At one point during the development of SAFEPAQ-II, the Mod type 5 modification only removed data points. Now this modification also ensures that a point at 60 MeV exits (20 MeV for a non-extended library). Prior to this it was necessary to add the 60 or 20 MeV point by means of a Mod type 16 modification. When comparing with an External database that used these additional Mod type 16 modifications, the list of reactions with different numbers of modifications can be very large. Most of these are actually not relevant as the External Mod type 16 is not required to be added to the Internal database. The Ignore final Mod type 16 mods check box in the Settings window (Figure 1) should be ticked if the External database contains these modifications.

Clicking the Tools|Compare|Pre-modifications… submenu item displays the Compare pre-modifications window shown in Figure 171. Prior to the window appearing the confirmation dialog shown in Figure 172 is displayed. This ensures that the comparison is being carried out between databases with the same reaction numbers. The window shows reactions where there are differences in the pre-modifications stored and that will be used to create Final. The values in External are shown. The contents of the grid can be copied or printed by clicking on the Copy or Print buttons respectively.

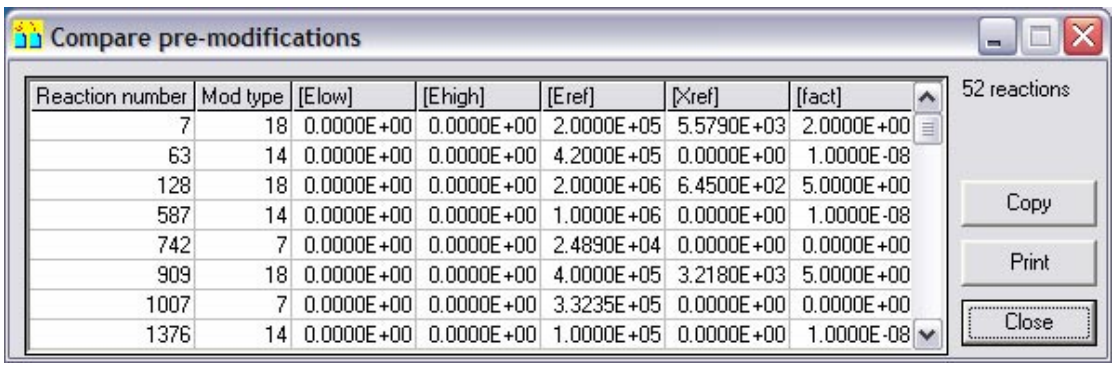


Figure 171. The Compare pre-modifications window.

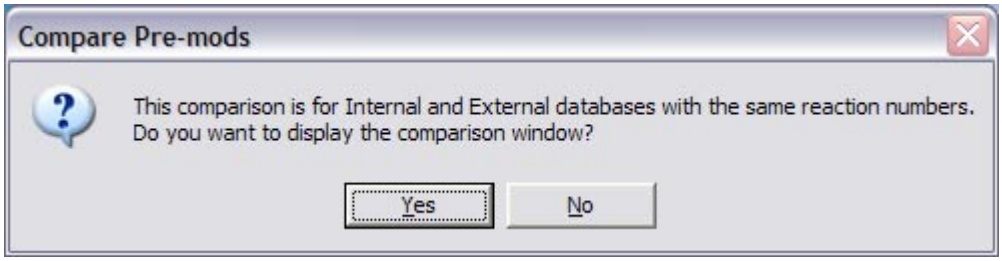
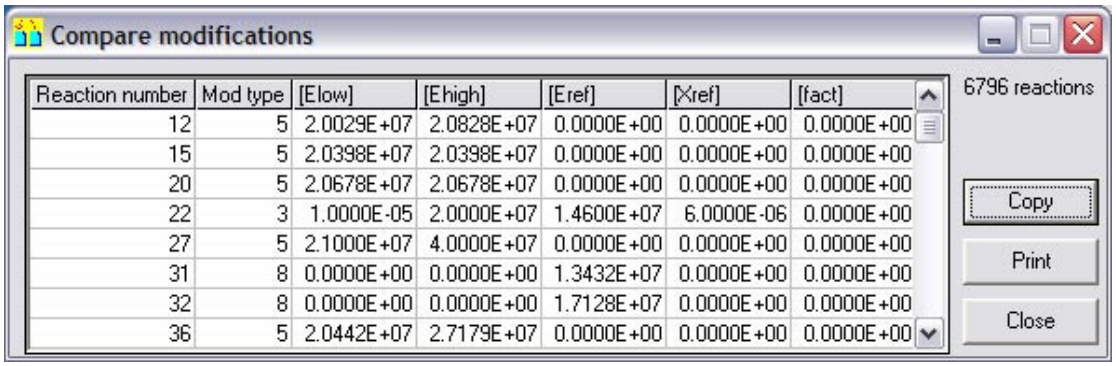

Compare Pre-mods
This comparison is for Internal and External databases with the same reaction numbers.
Do you want to display the comparison window?
Yes
No

Figure 172. The confirmation dialog prior to comparing pre-modifications.

Clicking the Tools|Compare|Modifications… submenu item displays the Compare modifications window shown in Figure 173. Prior to the window appearing the confirmation dialog similar to Figure 172 is displayed. This ensures that the comparison is being carried out between databases with the same reaction numbers. The window shows reactions where there are differences in the modifications stored and that will be used to create Final. The values in External are shown. The contents of the grid can be copied or printed by clicking on the Copy or Print buttons respectively.



Reaction number	Mod type	[Elow]	[Ehigh]	[Eref]	[Xref]	[fact]
12	5	2.0029E+07	2.0828E+07	0.0000E+00	0.0000E+00	0.0000E+00
15	5	2.0398E+07	2.0398E+07	0.0000E+00	0.0000E+00	0.0000E+00
20	5	2.0678E+07	2.0678E+07	0.0000E+00	0.0000E+00	0.0000E+00
22	3	1.0000E-05	2.0000E+07	1.4600E+07	6.0000E-06	0.0000E+00
27	5	2.1000E+07	4.0000E+07	0.0000E+00	0.0000E+00	0.0000E+00
31	8	0.0000E+00	0.0000E+00	1.3432E+07	0.0000E+00	0.0000E+00
32	8	0.0000E+00	0.0000E+00	1.7128E+07	0.0000E+00	0.0000E+00
36	5	2.0442E+07	2.7179E+07	0.0000E+00	0.0000E+00	0.0000E+00

Figure 173. The Compare modifications window.

Clicking the Tools|Compare|EXFOR… submenu item displays the Compare EXFOR window shown in Figure 174. This shows reactions where there are differences in the data sets selected for plotting from the EXFOR CD-ROMs and stored in the SAFEPAQ-II EXFOR database. The 'Use P' flag shows if the data entry is used for visualisation. The contents of the grid can be copied or printed by clicking on the Copy or Print buttons respectively.

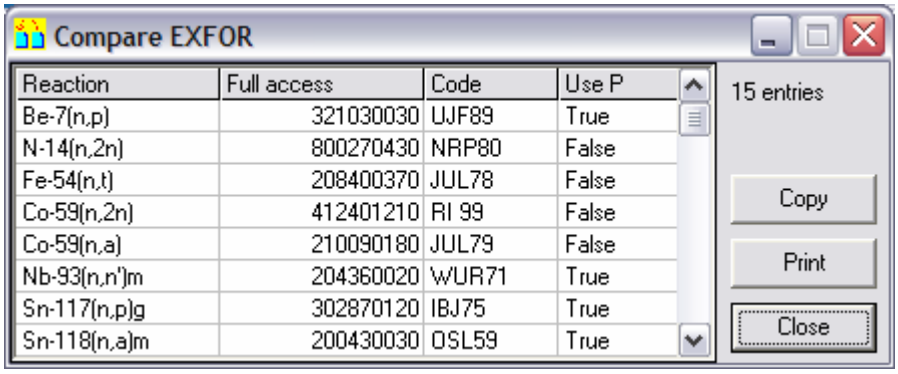


Figure 174. The Compare EXFOR window.

Clicking the Tools|Compare|Private EXFOR… submenu item displays the Compare Private EXFOR window shown in Figure 175. This shows reactions where there are differences in the Private EXFOR data sets stored in the SAFEPAQ-II EXFOR database. The contents of the grid can be copied or printed by clicking on the Copy or Print buttons respectively.

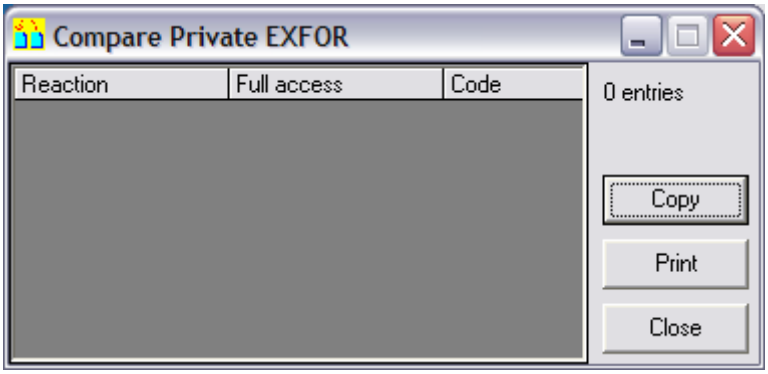


Figure 175. The Compare Private EXFOR window.

Clicking the Tools|Compare|Uncertainty data… submenu item displays the Compare uncertainty data window shown in Figure 176. This shows reactions where there are differences in the uncertainty data values (for non-threshold reactions). The values in External are shown. The contents of the grid can be copied or printed by clicking on the Copy or Print buttons respectively.

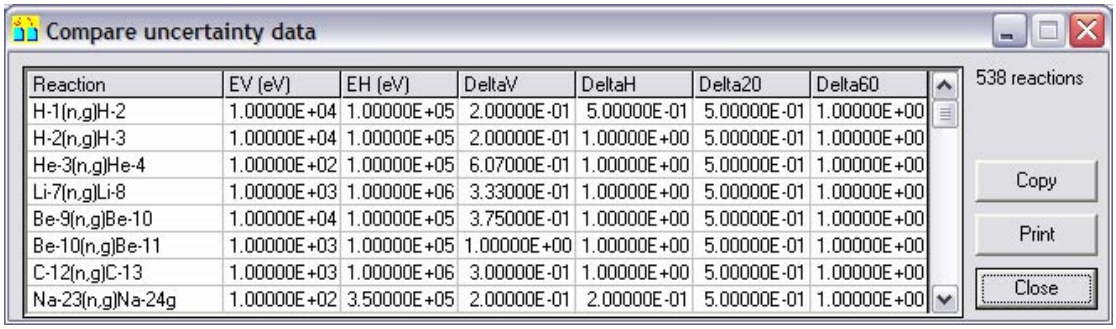


Figure 176. The Compare uncertainty data window.

Clicking the Tools|Compare|Threshold uncertainty data… submenu item displays the Compare threshold uncertainty data window shown in Figure 177. This shows reactions where there are differences in the uncertainty data values (for threshold reactions). The value in External is shown, and also an indication of whether it is a new entry or if the Delta value has been changed. The contents of the grid can be copied or printed by clicking on the Copy or Print buttons respectively.

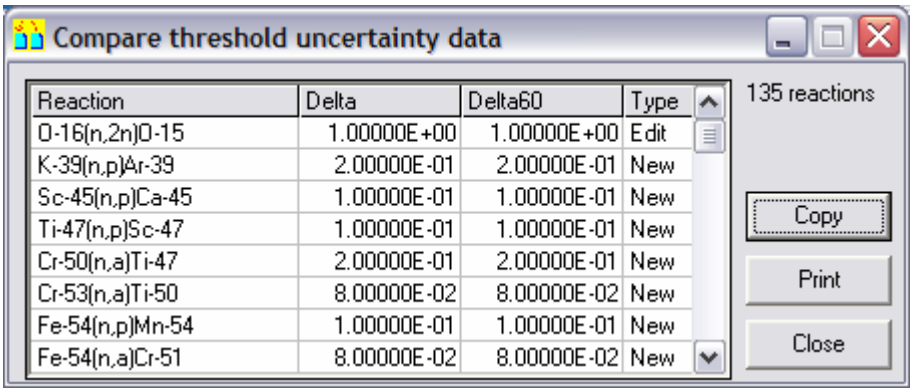


Figure 177. The Compare threshold uncertainty data window.

Clicking the Tools|Compare|Quality scores… submenu item displays the Compare Quality scores window shown in Figure 178. This shows reactions where there are differences in the scores. The scores in External and Internal and the number of different reactions are shown. The contents of the grid can be copied or printed by clicking on the Copy or Print buttons respectively.

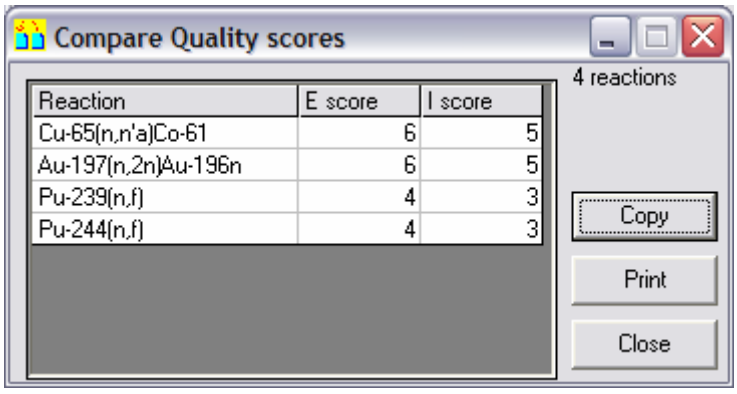


Figure 178. The Compare Quality scores window.

Using information from Figure 160 - Figure 178 enable changes to be made systematically to the Internal database that take into account the changes made in the External database.

The ability to view the Log in an External database is sometimes necessary in order to check on what changes have been made. This is possible by clicking on the Tools|View external Log… menu item that displays the Log window shown in Figure 6. In this case the title bar shows Log –

External and the contents of the External rather than Internal Log are shown.

A further way to compare with a previous EAF library has been available from EASY-2005. Clicking the Tools|Compare with previous EAF library… menu item displays the Compare with previous EAF library window shown in Figure 179. Prior to opening the window the confirmation dialog shown in Figure 180 is displayed. The Compare with previous EAF library window shows all the reactions in the current library and contains four tabs. The Source tab displays the data source and Quality score for the two libraries.

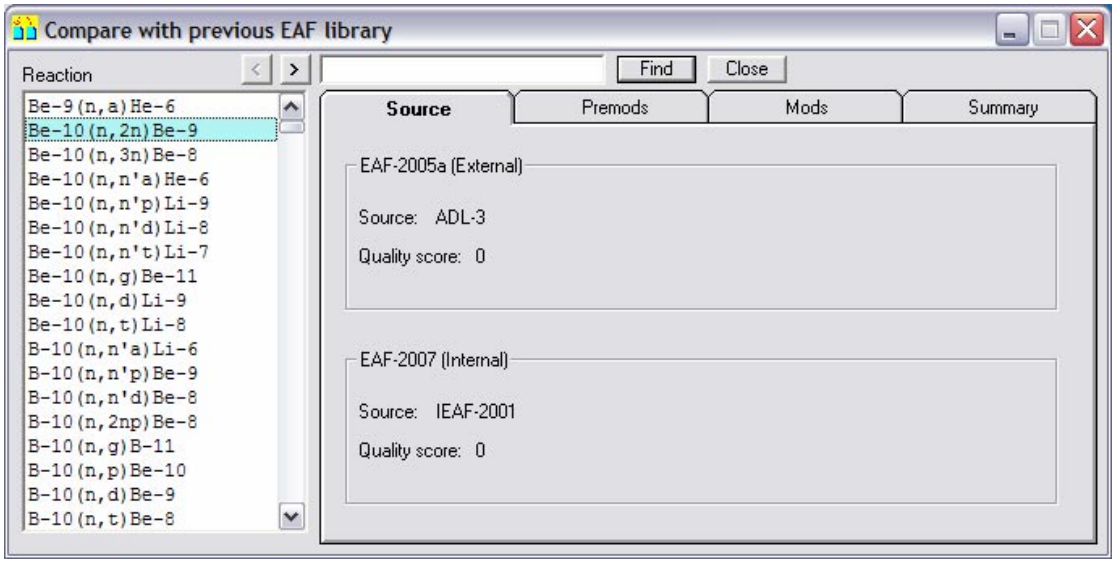


Figure 179. The Compare with previous EAF library window (Tab 1).

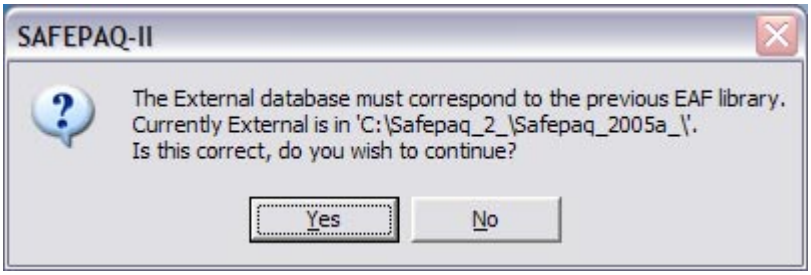

SAFEPAQ-II
The External database must correspond to the previous EAF library.
Currently External is in 'C:\Safepaq_2_\Safepaq_2005a_\'.
Is this correct, do you wish to continue?
Yes
No

Figure 180. The confirmation dialog prior to comparing with previous EAF library.

The second tab is displayed by clicking on the Premods tab; the result is shown in Figure 181. This shows details of the pre-modifications applied to the two libraries. The third tab is displayed by clicking on the Mods tab; the result is almost identical to Figure 181 except that modifications for the two libraries are shown.

The fourth tab is displayed by clicking on the Summary tab; the result is shown in Figure 182. This show the cross sections

at standard energies for the two libraries, the ratios and if available the values from experiment. The data grid can be printed to the default printer by clicking the Print button. The window can be closed from this tab by clicking the Close button, or the Close button at the top of the window. Note that if the Final summary values for the Internal database have not yet been calculated then a message to this effect is displayed in the window.

There are many reactions in the EAF libraries and to select a particular one the Find text box can be used. Enter a reaction string e.g. `Fe-56(n,p)` and clicking the Find button will display data for the selected reaction. To display reactions with high mass targets it is necessary to use the 'paging buttons': clicking > displays the next page and clicking < displays the previous page.

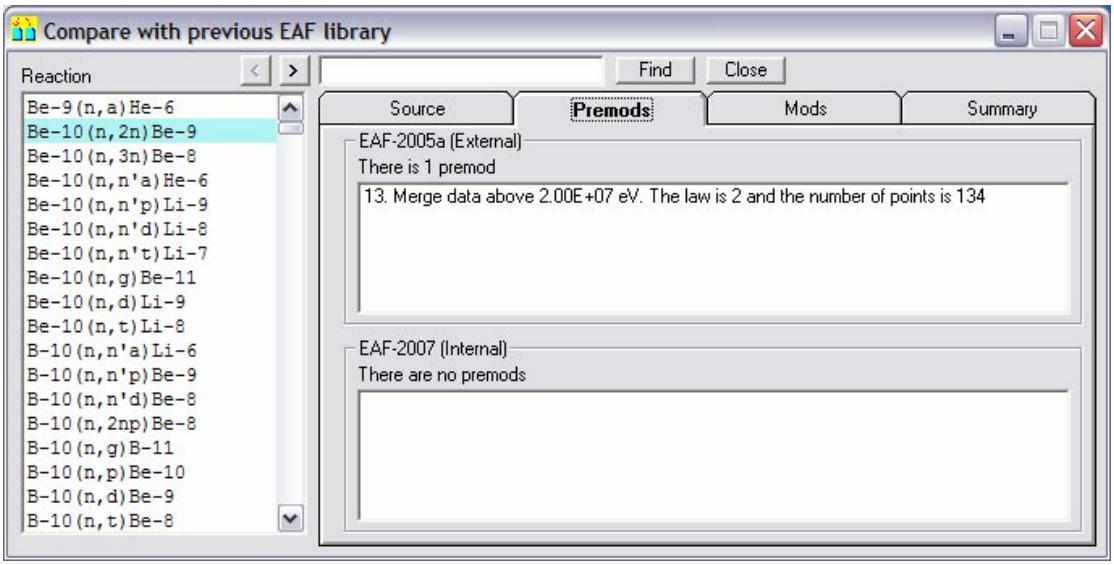


Figure 181. The Compare with previous EAF library window (Tab 2).

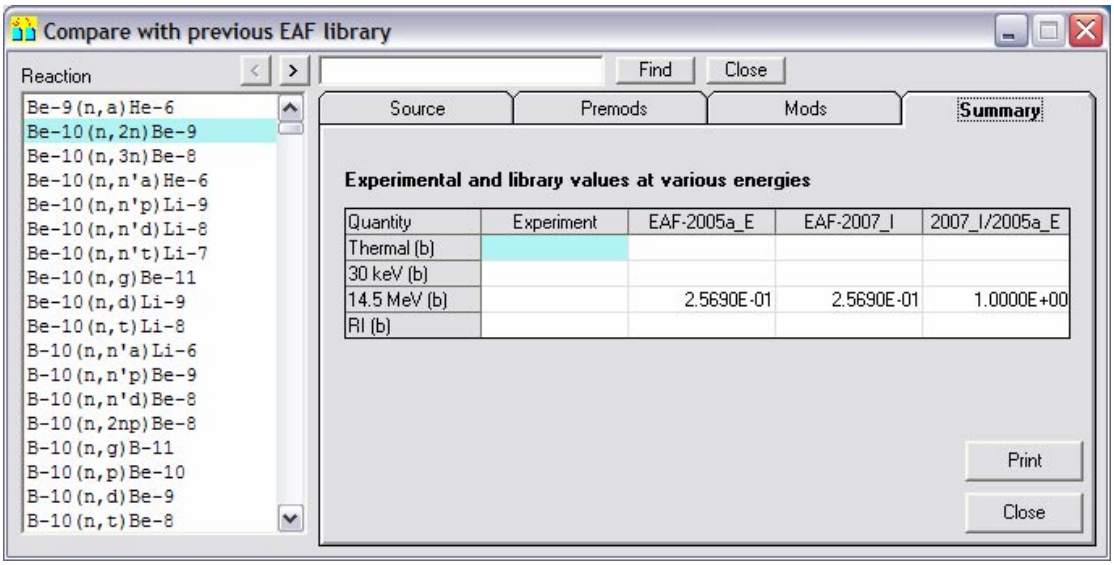


Figure 182. The Compare with previous EAF library window (Tab 4).

As discussed in Appendix 2, the use of linked tables in several of the databases used by SAFEPAQ-II can cause problems if databases are moved to another computer. To resolve such problems click on the Tools|Linked tables… menu item to display the Linked tables window shown in Figure 183.

There are two potential problems, firstly with Final and secondly with the various source databases. In Figure 183 the Final radio button is clicked, and clicking on the Find button displays in the text box the current location of the linked tables in Final. The list box shows all the tables with an indication of the linked ones. If the path is not valid then use the browse button (…) to open the standard Open dialog and select the correct *final_add.mdb* on the computer. Once this has been done the Change links button is enabled and clicking this will change all the links in *final.mdb* to the new specified location. The list box will show which tables have been relinked.

If the Data source radio button is clicked then a new dropdown list containing the names of all the data sources appears. Select the required source and click the Find button to show the location of *parameter.mdb* specified in the links. If links do not yet exist for the selected source, then a warning message is displayed. If the links exist then, as in the case of Final discussed above, these can be altered by clicking the browse (…) and Change links buttons. The window is closed by clicking the Close button.

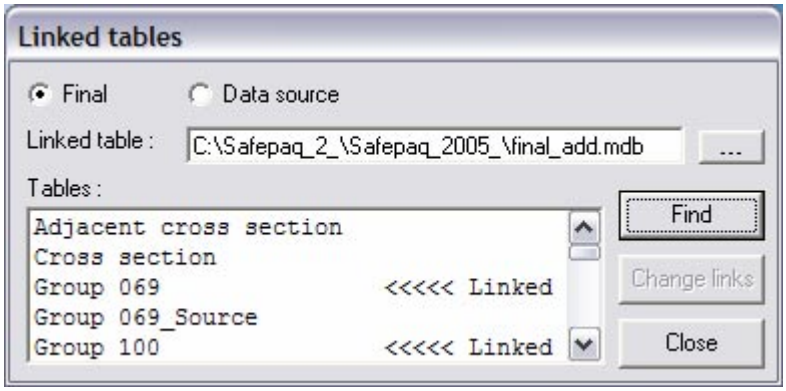
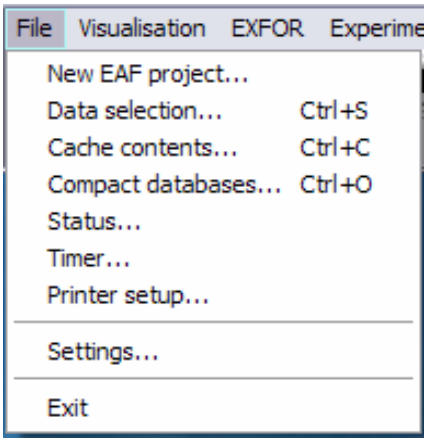


Figure 183. The Linked tables window.

Summary of menu items

The menu items that are available on the main SAFEPAQ-II window (Figure 2) are shown below. The page numbers where a description of the menu item can be found are given to the right of each menu item.



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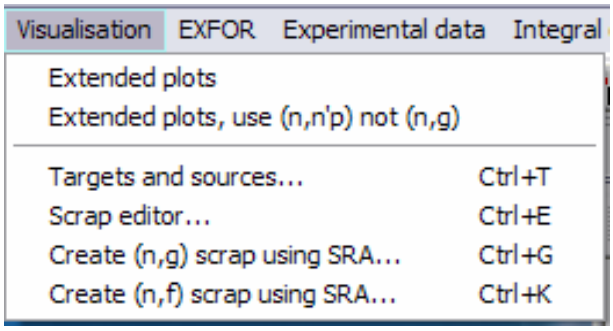

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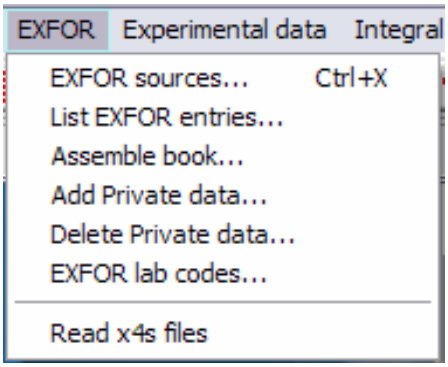

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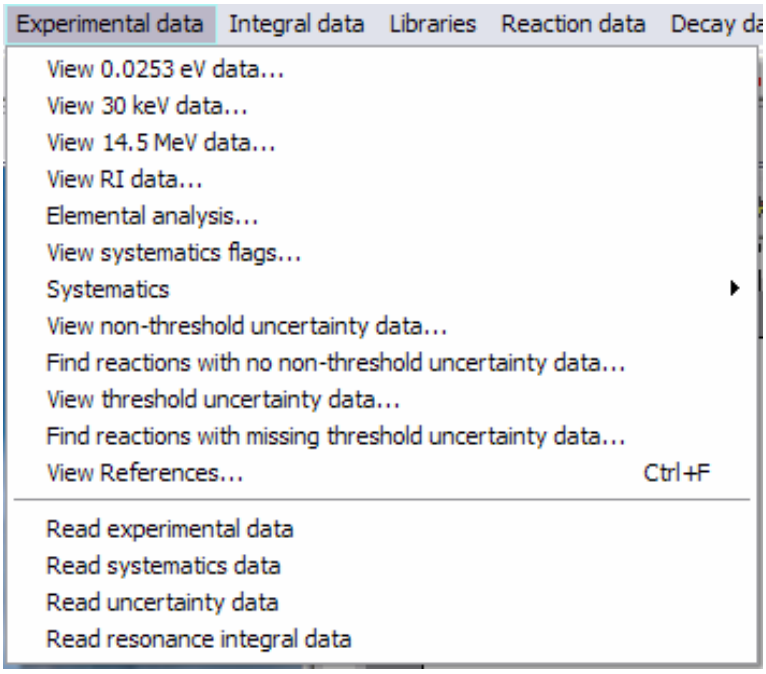

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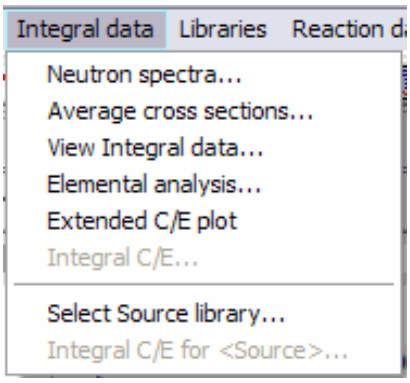

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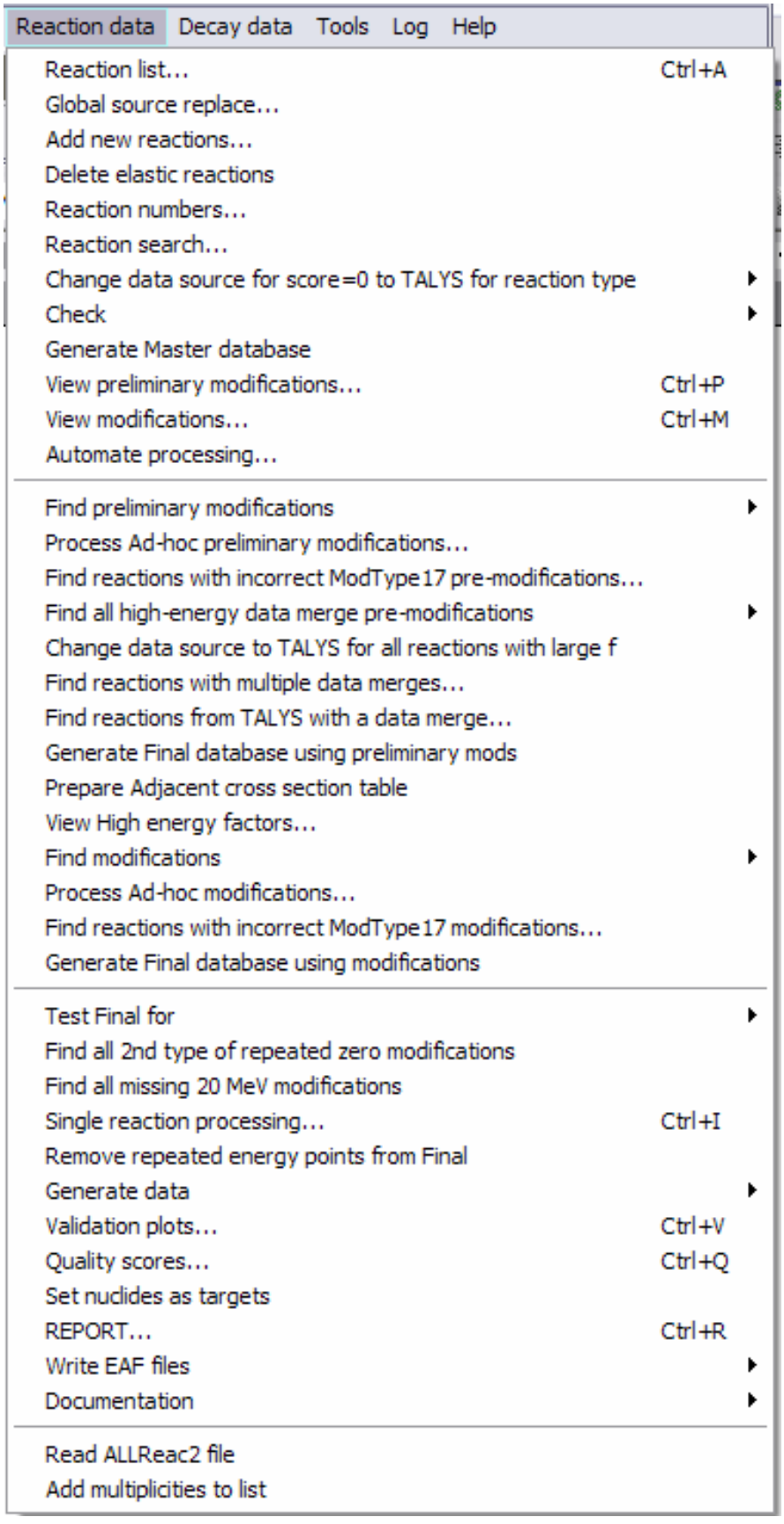
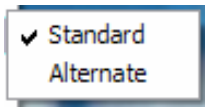

Reaction data
Decay data
Tools
Log
Help
Reaction list... Ctrl+A 75
Global source replace... 78
Add new reactions... 78
Delete elastic reactions 79
Reaction numbers... 79
Reaction search... 80
Change data source for score=0 to TALYS for reaction type See b
Check See c
Generate Master database 82
View preliminary modifications... Ctrl+P 84
View modifications... Ctrl+M 96
Automate processing... 91
Find preliminary modifications See d
Process Ad-hoc preliminary modifications... 87
Find reactions with incorrect ModType17 pre-modifications... 88
Find all high-energy data merge pre-modifications See e
Change data source to TALYS for all reactions with large f 89
Find reactions with multiple data merges... 90
Find reactions from TALYS with a data merge... 90
Generate Final database using preliminary mods 90
Prepare Adjacent cross section table 95
View High energy factors... 89
Find modifications See f
Process Ad-hoc modifications... 97
Find reactions with incorrect ModType17 modifications... 98
Generate Final database using modifications 98
Test Final for See g
Find all 2nd type of repeated zero modifications 100
Find all missing 20 MeV modifications 100
Single reaction processing... Ctrl+I 104
Remove repeated energy points from Final 108
Generate data See h
Validation plots... Ctrl+V 110
Quality scores... Ctrl+Q 103
Set nuclides as targets 115
REPORT... Ctrl+R 116
Write EAF files See i
Documentation See j
Read ALLReac2 file 119
Add multiplicities to list 119

a



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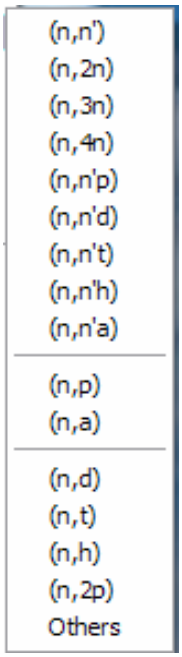
b



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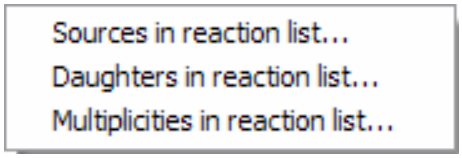

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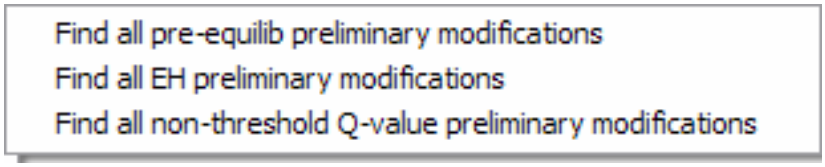
d


Find all pre-equilib preliminary modifications
Find all EH preliminary modifications
Find all non-threshold Q-value preliminary modifications

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e

Find all >20MeV data merge (TALYS) pre-modifications
Find all >20MeV data merge (IEAF) pre-modifications
Find all >50MeV data merge (TALYS) pre-modifications

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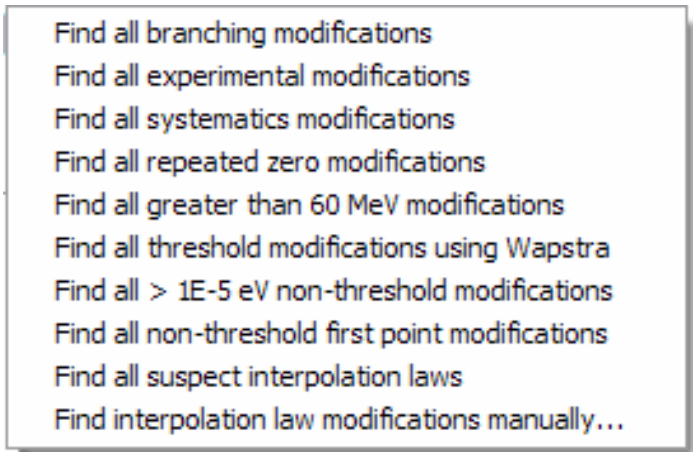
f


Find all branching modifications
Find all experimental modifications
Find all systematics modifications
Find all repeated zero modifications
Find all greater than 60 MeV modifications
Find all threshold modifications using Wapstra
Find all > 1E-5 eV non-threshold modifications
Find all non-threshold first point modifications
Find all suspect interpolation laws
Find interpolation law modifications manually...

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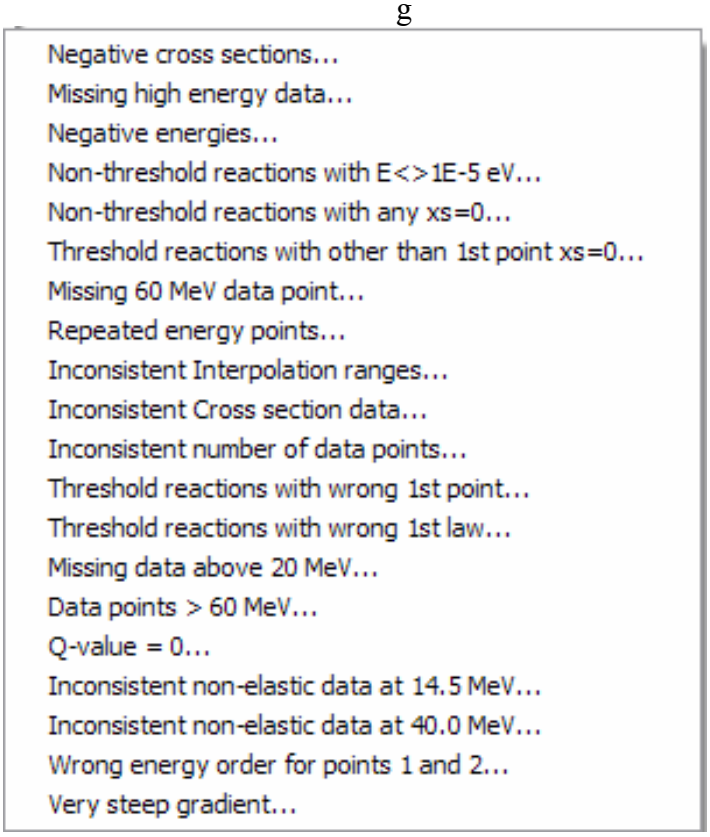
g


Negative cross sections...
Missing high energy data...
Negative energies...
Non-threshold reactions with E<>1E-5 eV...
Non-threshold reactions with any xs=0...
Threshold reactions with other than 1st point xs=0...
Missing 60 MeV data point...
Repeated energy points...
Inconsistent Interpolation ranges...
Inconsistent Cross section data...
Inconsistent number of data points...
Threshold reactions with wrong 1st point...
Threshold reactions with wrong 1st law...
Missing data above 20 MeV...
Data points > 60 MeV...
Q-value = 0...
Inconsistent non-elastic data at 14.5 MeV...
Inconsistent non-elastic data at 40.0 MeV...
Wrong energy order for points 1 and 2...
Very steep gradient...

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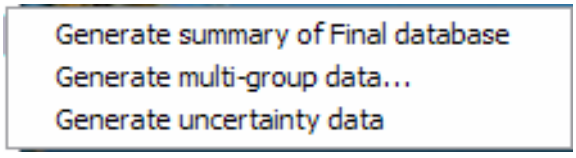

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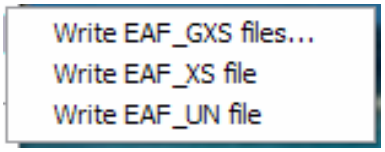
i



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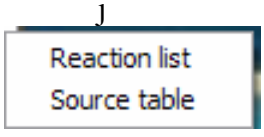
j



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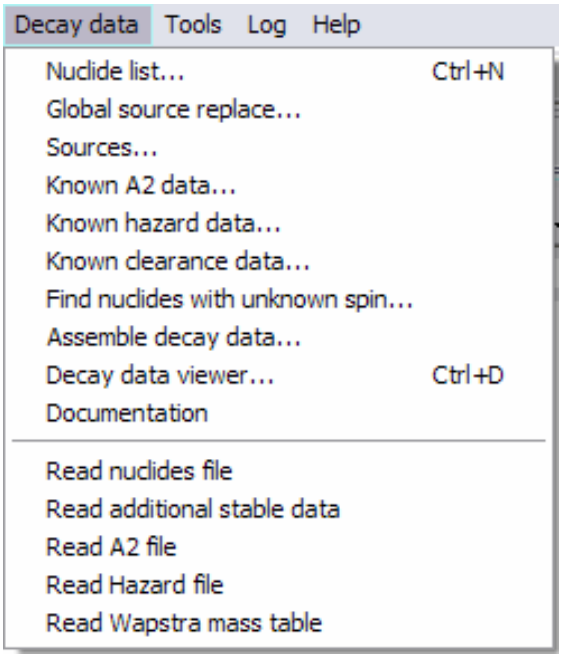

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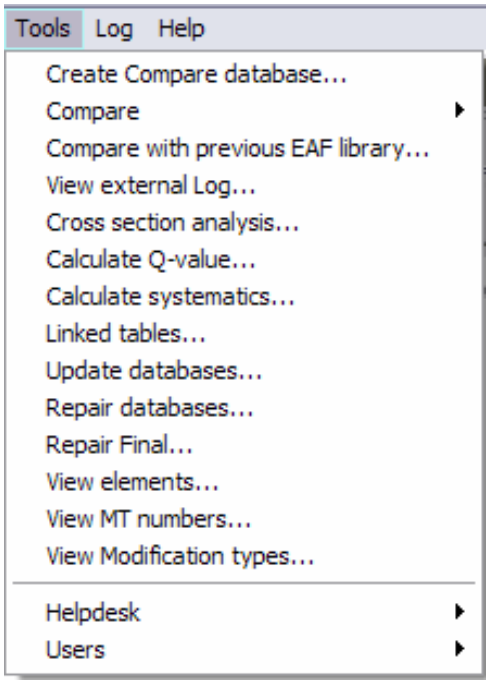

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See k
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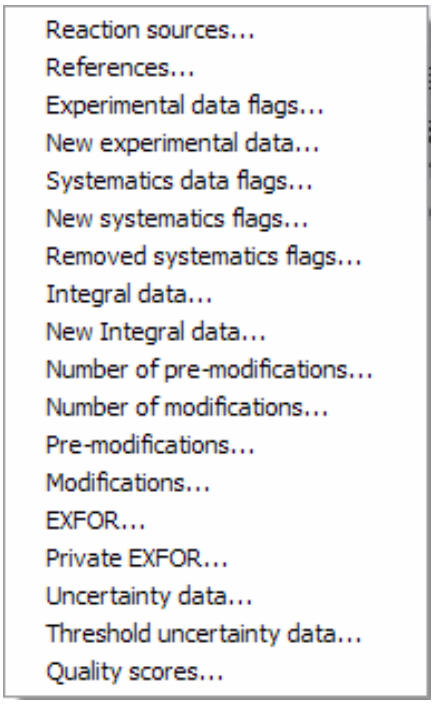
See l
See m

k



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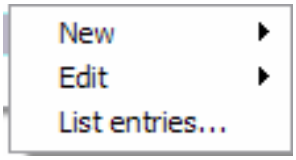

See n
See n
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m

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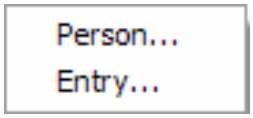
n



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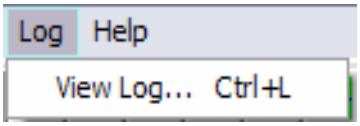

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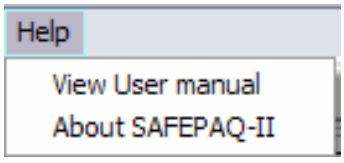

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9

References

[1] RA Forrest, *'FISPACT-2007: User manual'*, **UKAEA FUS 534**, 2007.

[2] JA Simpson, J-Ch Sublet and D Nierop, *'SYMPAL: User guide'*, **UKAEA FUS 356**, 1997.

[3] JA Simpson and J-Ch Sublet, *'SYMPAL: Utilities guide'*, **UKAEA FUS 357**, 1997.

[4] J-Ch Sublet, J Kopecky and RA Forrest, *'The European Activation File: EAF-99 cross section library'*, **UKAEA FUS 408**, 1998.

[5] RA Forrest and J-Ch Sublet, *'The European Activation File: EAF-99 decay data library'*, **UKAEA FUS 409**, 1998.

[6] RA Forrest and J-Ch Sublet, *'The European Activation File: EAF-99 biological, clearance and transport libraries'*, **UKAEA FUS 410**, 1998.

[7] RA Forrest and JA Simpson, *'SAFEPAQ: User manual'*, **UKAEA FUS 355**, 1997.

[8] Visual Numerics, Inc., *'PV-WAVE Foundation and PV-WAVE: Visual Exploration Documentation, Version 6'*, Boulder Colorado, USA, 1996.

[9] RA Forrest, *'The European Activation System: EASY-2007 overview'*, **UKAEA FUS 533**, 2007.

[10] RA Forrest, J Kopecky and J-Ch Sublet, *'The European Activation File: EAF-2007 neutron-induced cross section library'*, **UKAEA FUS 535**, 2007.

[11] RA Forrest, *'The European Activation File: EAF-2007 deuteron- and proton-induced cross section libraries'*, **UKAEA FUS 536**, 2007.

[12] RA Forrest, *'The European Activation File: EAF-2007 decay data library'*, **UKAEA FUS 537**, 2007.

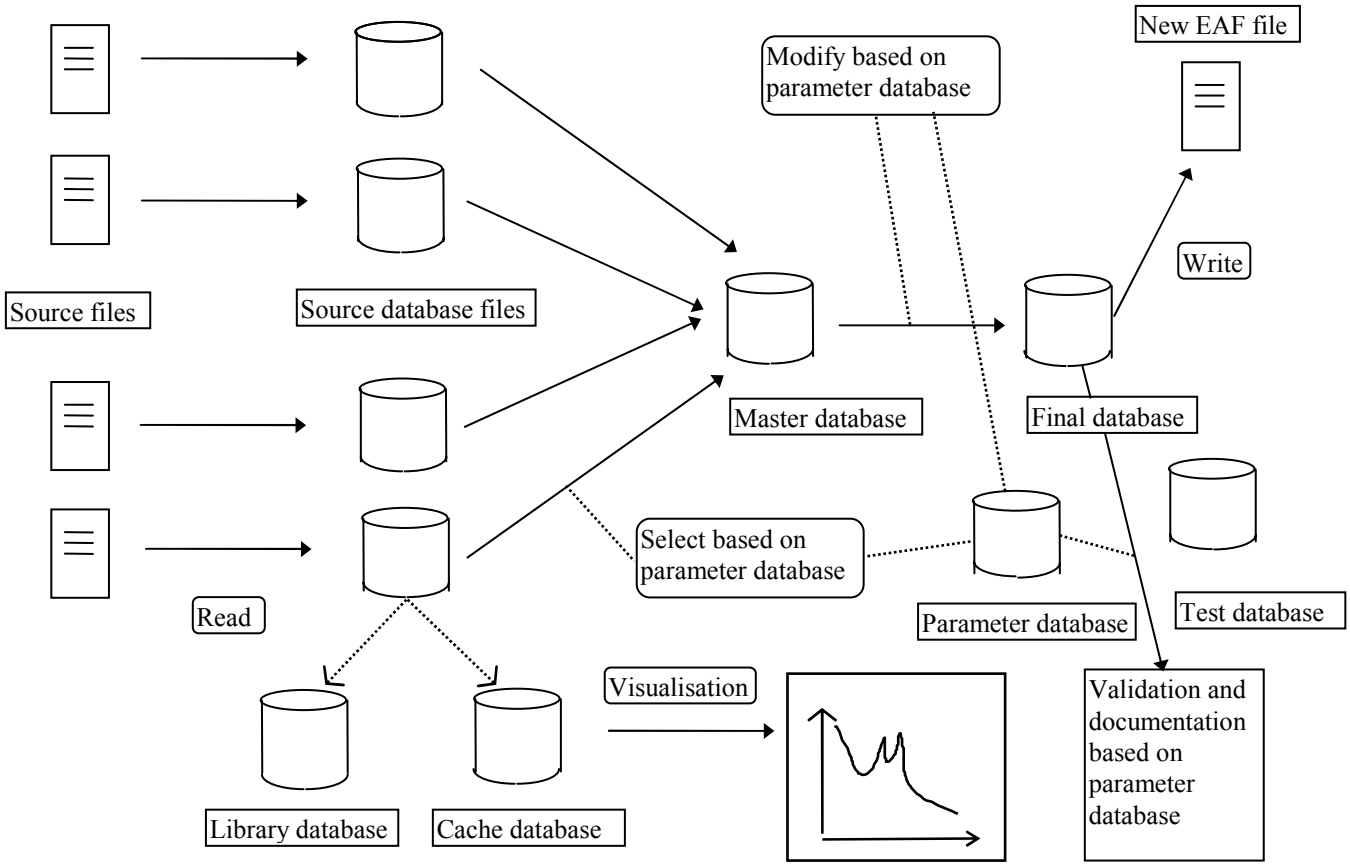
[13] RA Forrest, *'The European Activation File: EAF-2007 biological, clearance and transport libraries'*, **UKAEA FUS 538**, 2007.

[14] RA Forrest and J Kopecky, 'Statistical analysis of cross sections – A new tool for data validation', *Fus. Eng. Design*, **82**, 73-90, 2007.

[15] RA Forrest, 'Data requirements for neutron activation – Part I: Cross sections', *Fus. Eng. Design*, **81**, 2143-2156, 2006.

Appendix 1. SAFEPAQ-II design

1. Overall structure



2. Database design

The various source libraries each require a separate database to contain all the relevant data in a standard form. Each database is given a name <*source*>*.mdb*. The design of the database is given in *generic.mdb*, this database is copied and then renamed for each new database. Using the Documenter feature in Access the definitions of the tables in *generic.mdb* are given in Section 3. The fields in each table are shown.

The fields in each table are mostly self-explanatory, note that in the Reaction table the last six fields are given names taken directly from ENDF nomenclature. Note that wherever a floating-point data number is used it has a Double type and that Long integers are used in cases where more than one or two possibilities exist. Similar conventions are used in the design of all the remaining databases.

The *library.mdb* database contains the RawData table that describes the location of the source data file and the name of the database. A series of Boolean variables describe the format of the data and enable the reading and conversion to database

form to be achieved. The tables in the *library.mdb* database are defined in Section 4. The Reaction table is the same as that defined for *generic.mdb*.

The *parameter.mdb* database contains all the version dependent information. The tables in the *parameter.mdb* database are defined in Section 5.

The *master.mdb* database tables are very similar to those in *generic.mdb*, but also include information on the multiplicity of the source in addition to the actual multiplicity in the Reaction table. The tables in the *master.mdb* database are defined in Section 6.

The *cache.mdb* database tables are very similar to those in *master.mdb*, but also include information on the history of modifications made to the original data. The tables in the *cache.mdb* database are defined in Section 7.

The *final.mdb* database tables contain additional information on group data, and the suspect interpolation laws. The tables in the *final.mdb* database are defined in Section 8. Note that from EASY-2005 the *final_add.mdb* database contains all the *Group nnn* tables, except *Group 175F*. Final then contains links to these tables.

The *test.mdb* database tables are identical to *final.mdb*, except that the Adjacent cross section and suspect points tables are not present and AverageXS is added.

The *EXFOR.mdb* database is not shown in the diagram above. It contains information selected from the EXFOR CD-ROMs (see page 33) that are used for visualisation. The tables in the *EXFOR.mdb* database are defined in Section 9.

In addition to the tables present in each of the databases discussed above, extensive use is made of pre-compiled queries. Whenever data is selected from a database table, data in a record are amended or a new record is added this is achieved by calling a query from Visual Basic. In most cases various parameters are needed so that a particular query can be properly defined.

3. The definition of the generic.mdb database tables

Cross section

Name	Type	Size
Reaction number	Number (Long)	4
Point number	Number (Long)	4
Energy	Number (Double)	8
Cross section	Number (Double)	8

Details

Name	Type	Size
Name	Text	50
Calc_summary	Yes/No	1
Linked	Yes/No	1

Interpolation

Name	Type	Size
Reaction number	Number (Long)	4
Range number	Number (Integer)	2
Range limit	Number (Long)	4
Interpolation law	Number (Integer)	2

LibrarySummary

Name	Type	Size
Reaction number	Number (Long)	4
Cross section thermal	Number (Double)	8
Cross section 30keV	Number (Double)	8
Cross section 14MeV	Number (Double)	8
Resonance Integral	Number (Double)	8

Reaction

Name	Type	Size
Reaction number	Number (Long)	4
Source	Text	50
ZA target	Number (Long)	4
I target	Number (Integer)	2
ZA daughter	Number (Long)	4
I daughter	Number (Integer)	2
Multiplicity	Number (Integer)	2
MT	Number (Integer)	2
QM	Number (Double)	8
QI	Number (Double)	8
LR	Number (Integer)	2
NR	Number (Integer)	2
NP	Number (Long)	4

Systematics30Summary

Name	Type	Size
Reaction number	Number (Long)	4
ZA target	Number (Long)	4
I target	Number (Integer)	2
ZA daughter	Number (Long)	4
I daughter	Number (Integer)	2
MT	Number (Integer)	2
Cross section 30keV	Number (Double)	8
Systematics	Number (Double)	8

SystematicsSummary

Name	Type	Size
Reaction number	Number (Long)	4
ZA target	Number (Long)	4
I target	Number (Integer)	2
ZA daughter	Number (Long)	4
I daughter	Number (Integer)	2
MT	Number (Integer)	2
Cross section 14MeV	Number (Double)	8
Systematics	Number (Double)	8

Target

Name	Type	Size
Target number	Number (Integer)	2
ZA	Number (Long)	4
I	Number (Integer)	2

TotalLibrarySummary

Name	Type	Size
Reaction number	Number (Long)	4
Cross section thermal	Number (Double)	8
Cross section 30keV	Number (Double)	8
Cross section 14MeV	Number (Double)	8
Resonance Integral	Number (Double)	8

TotalReaction

Name	Type	Size
Reaction number	Number (Long)	4
ZA target	Number (Long)	4
I target	Number (Integer)	2
ZA daughter	Number (Long)	4
I daughter	Number (Integer)	2
Multiplicity	Number (Integer)	2
MT	Number (Integer)	2

4. The definition of the library.mdb *database tables*

Elements

Name	Type	Size
Z	Number (Integer)	2
Symbol	Text	2

MTvalues

Name	Type	Size
MT	Number (Integer)	2
Reaction name	Text	7

RawData

Name	Type	Size
Source	Text	50
Database name	Text	50
Path	Text	100
Strict ENDF	Yes/No	1
ADL-3	Yes/No	1
JENDL	Yes/No	1
EAF	Yes/No	1
XY Table	Yes/No	1
Version 6	Yes/No	1
MF2	Yes/No	1
MF4	Yes/No	1
MF32	Yes/No	1
MF33	Yes/No	1
1 material per file	Yes/No	1
Header	Yes/No	1
FEND	Yes/No	1
MEND	Yes/No	1
TEND	Yes/No	1
IEAF	Yes/No	1
MF6	Yes/No	1
IPType	Text	10
Derived	Yes/No	1
ANITA	Yes/No	1

Reaction

Name	Type	Size
Reaction number	Number (Long)	4
Source	Text	50
ZA target	Number (Long)	4
I target	Number (Integer)	2
ZA daughter	Number (Long)	4
I daughter	Number (Integer)	2
Multiplicity	Number (Integer)	2
MT	Number (Integer)	2
QM	Number (Double)	8
QI	Number (Double)	8
LR	Number (Integer)	2
NR	Number (Integer)	2
NP	Number (Long)	4

Source

Name	Type	Size
Source ID	Number (Integer)	2
Source	Text	50
Number targets	Number (Integer)	2
Number reactions	Number (Long)	4
Number n	Number (Long)	4
Number 2n	Number (Long)	4
Number 3n	Number (Long)	4
Number f	Number (Long)	4
Number na	Number (Long)	4
Number 2na	Number (Long)	4
Number np	Number (Long)	4
Number n2a	Number (Long)	4
Number nd	Number (Long)	4
Number nt	Number (Long)	4
Number nh	Number (Long)	4
Number 4n	Number (Long)	4
Number 2np	Number (Long)	4
Number g	Number (Long)	4
Number p	Number (Long)	4
Number d	Number (Long)	4
Number t	Number (Long)	4
Number h	Number (Long)	4
Number a	Number (Long)	4
Number 2a	Number (Long)	4
Number 2p	Number (Long)	4

5. The definition of the parameter.mdb *database tables*

A2_IAEA

Name	Type	Size
ZA	Number (Long)	4
Isom	Number (Integer)	2
A2	Number (Single)	4

AdditionalData

Name	Type	Size
Add number	Number (Long)	4
Point number	Number (Long)	4
Energy	Number (Double)	8
Cross section	Number (Double)	8

AverageXS

Name	Type	Size
Reaction number	Number (Long)	4
Spectrum ID	Number (Integer)	2
Average XS	Number (Double)	8

AverageXS_Source

Name	Type	Size
Reaction number	Number (Long)	4
Source ID	Number (Integer)	2
Spectrum ID	Number (Integer)	2
Average XS	Number (Double)	8

bound_069

Name	Type	Size
Group number	Number (Integer)	2
Energy	Number (Double)	8
Weight	Number (Integer)	2

bound_100

Name	Type	Size
Group number	Number (Integer)	2
Energy	Number (Double)	8
Weight	Number (Integer)	2

bound_172

Name	Type	Size
Group number	Number (Integer)	2
Energy	Number (Double)	8
Weight fission	Number (Integer)	2
Weight fusion	Number (Integer)	2

bound_175

Name	Type	Size
Group number	Number (Integer)	2
Energy	Number (Double)	8
Weight	Number (Integer)	2

bound_211

Name	Type	Size
Group number	Number (Integer)	2
Energy	Number (Double)	8

bound_315

Name	Type	Size
Group number	Number (Integer)	2
Energy	Number (Double)	8
Weight fission	Number (Integer)	2
Weight fusion	Number (Integer)	2

bound_351

Name	Type	Size
Group number	Number (Integer)	2
Energy	Number (Double)	8

Boundary

Name	Type	Size
subfile	Number (Integer)	2
ZA	Number (Long)	4
I	Number (Integer)	2

BranchingStatus

Name	Type	Size
Reaction number	Number (Long)	4

All branching	Yes/No	1
Low branching	Yes/No	1
Mid branching	Yes/No	1
High branching	Yes/No	1
Mid factor	Number (Double)	8

BRData

Name	Type	Size
Isomer spin	Number (Single)	4
BR_1	Number (Double)	8
BR_2	Number (Double)	8
BR_3	Number (Double)	8

Clearance_IAEA

Name	Type	Size
ZA	Number (Long)	4
Isom	Number (Integer)	2
Clearance	Number (Single)	4

Clearance_IAEA_old

Name	Type	Size
ZA	Number (Long)	4
Isom	Number (Integer)	2
Clearance	Number (Single)	4

DecayData

Name	Type	Size
Nuclide number	Number (Integer)	2
Name	Text	7
Source	Text	50
ZA	Number (Long)	4
AWR	Number (Double)	8
MAT	Number (Integer)	2
ELIS	Number (Double)	8
STA	Number (Integer)	2
LISO	Number (Integer)	2
THALF	Number (Double)	8
D_THALF	Number (Double)	8
EA	Number (Double)	8
D_EA	Number (Double)	8
EB	Number (Double)	8
D_EB	Number (Double)	8
EG	Number (Double)	8
D_EG	Number (Double)	8
SPI	Number (Single)	4
PAR	Number (Integer)	2
NDK	Number (Integer)	2
RTYP_1	Number (Single)	4
RTYP_2	Number (Single)	4
RTYP_3	Number (Single)	4
RTYP_4	Number (Single)	4
RFS_1	Number (Integer)	2
RFS_2	Number (Integer)	2
RFS_3	Number (Integer)	2
RFS_4	Number (Integer)	2
Q_1	Number (Double)	8
Q_2	Number (Double)	8
Q_3	Number (Double)	8
Q_4	Number (Double)	8
D_Q_1	Number (Double)	8
D_Q_2	Number (Double)	8
D_Q_3	Number (Double)	8
D_Q_4	Number (Double)	8
BR_1	Number (Double)	8
BR_2	Number (Double)	8
BR_3	Number (Double)	8
BR_4	Number (Double)	8
D_BR_1	Number (Double)	8
D_BR_2	Number (Double)	8

D_BR_3	Number (Double)	8
D_BR_4	Number (Double)	8
A2	Number (Double)	8
A2SOURCE	Text	50
CING	Number (Double)	8
CINH	Number (Double)	8
HAZSRC	Text	50
Clearance	Number (Double)	8
ClearSource	Text	50

Decaydata sources

Name	Type	Size
Source	Text	50
Header	Number (Integer)	2

Details

Name	Type	Size
Name	Text	50
Description	Text	255
Start Mod	Number (Long)	4
PreModMaxAddnum	Number (Long)	4
DecayDB	Yes/No	1
MasterDB	Yes/No	1
FoundPM	Yes/No	1
FinalDB_PM	Yes/No	1
AdjacentTable	Yes/No	1
FoundM_BR	Yes/No	1
FoundM_Exp	Yes/No	1
FoundM_Sys	Yes/No	1
FoundM_Zero	Yes/No	1
FoundM_20	Yes/No	1
FoundM_Thresh	Yes/No	1
FoundM_LowE	Yes/No	1
FoundM_NonThresh	Yes/No	1
FoundM_Suspect	Yes/No	1
FinalDB_M	Yes/No	1
Calc_Summary	Yes/No	1
Calc_069	Yes/No	1
Calc_100	Yes/No	1
Calc_172	Yes/No	1
Calc_175	Yes/No	1
Calc_211	Yes/No	1
Calc_315	Yes/No	1
Calc_351	Yes/No	1
Calc_Uncert	Yes/No	1
Write_GXS	Yes/No	1
Write_XS	Yes/No	1
Write_UN	Yes/No	1

Elements

Name	Type	Size
Z	Number (Integer)	2
Symbol	Text	2

Error factors

Name	Type	Size
MT	Number (Integer)	2
f	Number (Double)	8
name	Text	50

ExpData

Name	Type	Size
Exp number	Number (Long)	4
ZA	Number (Long)	4
I	Number (Integer)	2
ZAD	Number (Long)	4
ID	Number (Integer)	2
MT	Number (Integer)	2

Use B	Yes/No	1
Use R	Yes/No	1
Use V	Yes/No	1
Energy	Number (Double)	8
Cross section	Number (Double)	8
Delta Cross section	Number (Double)	8
Source	Text	5

FinalSummary

Name	Type	Size
Reaction number	Number (Long)	4
Cross section thermal	Number (Double)	8
Cross section 30keV	Number (Double)	8
Cross section 14MeV	Number (Double)	8
Resonance Integral	Number (Double)	8
Cross section 40MeV	Number (Double)	8

GammaGamma

Name	Type	Size
A	Number (Integer)	2
Width	Number (Double)	8

HighEnergyFactors

Name	Type	Size
Reaction number	Number (Long)	4
Factor	Number (Double)	8

Important_2003

Name	Type	Size
Reaction number	Number (Long)	4
ZA	Number (Long)	4
I	Number (Integer)	2
MT	Number (Integer)	2
ZAD	Number (Long)	4
ID	Number (Integer)	2

Integral Data

Name	Type	Size
Exp number	Number (Long)	4
ZA	Number (Long)	4
I	Number (Integer)	2
ZAD	Number (Long)	4
ID	Number (Integer)	2
MT	Number (Integer)	2
Use	Yes/No	1
Spectrum ID	Number (Integer)	2
Cross section	Number (Double)	8
Delta Cross section	Number (Double)	8
Source	Text	5

InterpMods

Name	Type	Size
Reaction number	Number (Long)	4
Source	Text	50
E low	Number (Double)	8
E high	Number (Double)	8
E ref	Number (Double)	8
X ref	Number (Double)	8
factor	Number (Double)	8
Add number	Number (Long)	4
Exp number	Number (Long)	4
Comment	Text	50

KnownHazards

Name	Type	Size
ZA	Number (Long)	4
Isom	Number (Integer)	2
CEDE_Ing	Number (Single)	4
CEDE_Inh	Number (Single)	4
Source	Text	7

LevelDensity

Name	Type	Size
Nucleon	Number (Integer)	2
a	Number (Double)	8
PZ	Number (Double)	8
PN	Number (Double)	8

LineData

Name	Type	Size
Nuclide number	Number (Integer)	2
STYP	Number (Byte)	1
RTYP	Number (Single)	4
Energy	Number (Double)	8
DEnergy	Number (Double)	8
Intensity	Number (Double)	8
DIntensity	Number (Double)	8

Log

Name	Type	Size
Date_Time	Date/Time	8
Action	Text	100
Comment	Text	100
Type	Number (Byte)	1
UserID	Text	3

ModAdhocAdd

Name	Type	Size
Mod number	Number (Long)	4
Reaction number	Number (Long)	4

ModAdhocDel

Name	Type	Size
Mod number	Number (Long)	4
Reaction number	Number (Long)	4
Mod type	Number (Integer)	2
E low	Number (Double)	8
E high	Number (Double)	8
E ref	Number (Double)	8
X ref	Number (Double)	8
factor	Number (Double)	8

ModDetails

Name	Type	Size
Mod type	Number (Integer)	2
Action	Text	30
Specification	Text	200

Modification

Name	Type	Size
Mod number	Number (Long)	4
Mod type	Number (Integer)	2
E low	Number (Double)	8
E high	Number (Double)	8

E ref	Number (Double)	8
X ref	Number (Double)	8
factor	Number (Double)	8
Add number	Number (Long)	4
Exp number	Number (Long)	4
Kind	Number (Byte)	1
Comment	Text	50

ModSummary

Name	Type	Size
Reaction number	Number (Long)	4
Number Mods	Number (Integer)	2
Mod 1	Number (Long)	4
Mod 2	Number (Long)	4
Mod 3	Number (Long)	4
Mod 4	Number (Long)	4
Mod 5	Number (Long)	4
Mod 6	Number (Long)	4
Mod 7	Number (Long)	4
Mod 8	Number (Long)	4
Mod 9	Number (Long)	4
Mod 10	Number (Long)	4

NucProperties

Name	Type	Size
ZA	Number (Long)	4
Isom	Number (Integer)	2
MAT	Number (Integer)	2
AWR	Number (Double)	8
ELIS	Number (Double)	8
SPI	Number (Single)	4
PAR	Number (Integer)	2

NucSummary

Name	Type	Size
ZA	Number (Long)	4
Isom	Number (Integer)	2
Target	Yes/No	1
Source	Text	50

PreModAdhocAdd

Name	Type	Size
Mod number	Number (Long)	4
Reaction number	Number (Long)	4

PreModAdhocDel

Name	Type	Size
Mod number	Number (Long)	4
Reaction number	Number (Long)	4
Mod type	Number (Integer)	2
E low	Number (Double)	8
E high	Number (Double)	8
E ref	Number (Double)	8
X ref	Number (Double)	8
factor	Number (Double)	8

PreModification

Name	Type	Size
Mod number	Number (Long)	4
Mod type	Number (Integer)	2
E low	Number (Double)	8
E high	Number (Double)	8
E ref	Number (Double)	8
X ref	Number (Double)	8

factor	Number (Double)	8
Add number	Number (Long)	4
Exp number	Number (Long)	4
Kind	Number (Byte)	1
Comment	Text	50

PreModSummary

Name	Type	Size
Reaction number	Number (Long)	4
Number Mods	Number (Integer)	2
Mod 1	Number (Long)	4
Mod 2	Number (Long)	4
Mod 3	Number (Long)	4
Mod 4	Number (Long)	4
Mod 5	Number (Long)	4
Mod 6	Number (Long)	4
Mod 7	Number (Long)	4
Mod 8	Number (Long)	4
Mod 9	Number (Long)	4
Mod 10	Number (Long)	4

ReacSummary

Name	Type	Size
Reaction number	Number (Long)	4
ZA target	Number (Long)	4
I target	Number (Integer)	2
ZA daughter	Number (Long)	4
I daughter	Number (Integer)	2
Multiplicity	Number (Integer)	2
MT	Number (Integer)	2
Source	Text	50
Status	Number (Byte)	1
Score	Number (Byte)	1

ReactionType

Name	Type	Size
MT	Number (Integer)	2
Reaction	Text	8

Reference

Name	Type	Size
Source	Text	5
Reference	Text	250

RIData

Name	Type	Size
RI number	Number (Long)	4
ZA	Number (Long)	4
I	Number (Integer)	2
ZAD	Number (Long)	4
ID	Number (Integer)	2
MT	Number (Integer)	2
Use B	Yes/No	1
Use R	Yes/No	1
Use V	Yes/No	1
RI	Number (Double)	8
Delta RI	Number (Double)	8

SourceData

Name	Type	Size
Reaction number	Number (Long)	4
Source I daughter	Number (Integer)	2
Source Multiplicity	Number (Integer)	2
Source MT	Number (Integer)	2

Spectra

Name	Type	Size
ID	Number (Integer)	2
Group number	Number (Integer)	2
Flux	Number (Double)	8

SpectraSummary

Name	Type	Size
ID	Number (Integer)	2
Name	Text	20
Structure	Number (Integer)	2
Groups	Number (Integer)	2
Description	Text	100
Reference	Text	10

StablesData

Name	Type	Size
ZA	Number (Long)	4
I	Number (Integer)	2
Spin	Number (Single)	4
Parity	Number (Integer)	2
Mass	Number (Double)	8
Abundance	Number (Double)	8

SystData

Name	Type	Size
Syst number	Number (Long)	4
ZA	Number (Long)	4
I	Number (Integer)	2
ZAD	Number (Long)	4
ID	Number (Integer)	2
MT	Number (Integer)	2
Use B	Yes/No	1
Use R	Yes/No	1

Syst30Data

Name	Type	Size
Syst number	Number (Long)	4
ZA	Number (Long)	4
I	Number (Integer)	2
ZAD	Number (Long)	4
ID	Number (Integer)	2
MT	Number (Integer)	2
Use B	Yes/No	1
Use R	Yes/No	1

SystematicsSummary

Name	Type	Size
Reaction number	Number (Long)	4
ZA target	Number (Long)	4
I target	Number (Integer)	2
ZA daughter	Number (Long)	4
I daughter	Number (Integer)	2
MT	Number (Integer)	2
Cross section 14MeV	Number (Double)	8
Systematics	Number (Double)	8
Systematics_alt	Number (Double)	8

Systematics20Summary

Name	Type	Size
Reaction number	Number (Long)	4
ZA target	Number (Long)	4
I target	Number (Integer)	2
ZA daughter	Number (Long)	4
I daughter	Number (Integer)	2
MT	Number (Integer)	2
Cross section 20MeV	Number (Double)	8
Systematics	Number (Double)	8

Systematics30Summary

Name	Type	Size
Reaction number	Number (Long)	4
ZA target	Number (Long)	4
I target	Number (Integer)	2
ZA daughter	Number (Long)	4
I daughter	Number (Integer)	2
MT	Number (Integer)	2
Cross section 30keV	Number (Double)	8
Systematics	Number (Double)	8

TotalFinalSummary

Name	Type	Size
Reaction number	Number (Long)	4
Cross section thermal	Number (Double)	8
Cross section 30keV	Number (Double)	8
Cross section 14MeV	Number (Double)	8
Resonance Integral	Number (Double)	8
Cross section 40MeV	Number (Double)	8

TotalFinalUncert

Name	Type	Size
Reaction number	Number (Long)	4
Group number	Number (Long)	4
Energy	Number (Double)	8
DeltaSquared	Number (Double)	8

TotalReacSummary

Name	Type	Size
Reaction number	Number (Long)	4
ZA target	Number (Long)	4
I target	Number (Integer)	2
ZA daughter	Number (Long)	4
I daughter	Number (Integer)	2
Multiplicity	Number (Integer)	2
MT	Number (Integer)	2
Source	Text	50

UncertData

Name	Type	Size
Uncert number	Number (Long)	4
ZA	Number (Long)	4
I	Number (Integer)	2
ZAD	Number (Long)	4
ID	Number (Integer)	2
MT	Number (Integer)	2
Use B	Yes/No	1
Use R	Yes/No	1
Use V	Yes/No	1
EV	Number (Double)	8
EH	Number (Double)	8
DeltaV	Number (Double)	8
DeltaH	Number (Double)	8
Delta20	Number (Double)	8
Delta60	Number (Double)	8

UncertDataThreshold

Name	Type	Size
Uncert number	Number (Long)	4
ZA	Number (Long)	4
I	Number (Integer)	2
ZAD	Number (Long)	4
ID	Number (Integer)	2
MT	Number (Integer)	2
Use B	Yes/No	1
Use R	Yes/No	1
Use V	Yes/No	1
VAR	Number (Double)	8
Delta60	Number (Double)	8

WapstraMass

Name	Type	Size
ZA	Number (Long)	4
Mass	Number (Double)	8

6. The definition of the master.mdb database tables

Cross section

Name	Type	Size
Reaction number	Number (Long)	4
Point number	Number (Long)	4
Energy	Number (Double)	8
Cross section	Number (Double)	8

Interpolation

Name	Type	Size
Reaction number	Number (Long)	4
Range number	Number (Integer)	2
Range limit	Number (Long)	4
Interpolation law	Number (Integer)	2

Reaction

Name	Type	Size
Reaction number	Number (Long)	4
Source	Text	50
ZA target	Number (Long)	4
I target	Number (Integer)	2
ZA daughter	Number (Long)	4
I daughter	Number (Integer)	2
Multiplicity	Number (Integer)	2
Source I daughter	Number (Integer)	2
Source Multiplicity	Number (Integer)	2
MT	Number (Integer)	2
QM	Number (Double)	8
QI	Number (Double)	8
LR	Number (Integer)	2
NR	Number (Integer)	2
NP	Number (Long)	4

Target

Name	Type	Size
Target number	Number (Long)	4
ZA	Number (Long)	4
I	Number (Integer)	2

7. The definition of the cache.mdb database tables

Cross section

Name	Type	Size
Reaction number	Number (Long)	4
Point number	Number (Long)	4
Energy	Number (Double)	8
Cross section	Number (Double)	8

Interpolation

Name	Type	Size
Reaction number	Number (Long)	4
Range number	Number (Integer)	2
Range limit	Number (Long)	4
Interpolation law	Number (Integer)	2

Reaction

Name	Type	Size
Reaction number	Number (Long)	4
Source	Text	50
ZA target	Number (Long)	4
I target	Number (Integer)	2
ZA daughter	Number (Long)	4
I daughter	Number (Integer)	2
Multiplicity	Number (Integer)	2
Source I daughter	Number (Integer)	2
Source Multiplicity	Number (Integer)	2
MT	Number (Integer)	2
QM	Number (Double)	8
QI	Number (Double)	8
LR	Number (Integer)	2
NR	Number (Integer)	2
NP	Number (Long)	4
History	Text	255

Target

Name	Type	Size
Target number	Number (Integer)	2
ZA	Number (Long)	4
I	Number (Integer)	2

8. The definition of the final.mdb *database tables*

Adjacent cross section

Name	Type	Size
Reaction number	Number (Long)	4
Point number	Number (Long)	4
Energy	Number (Double)	8
Cross section	Number (Double)	8
Next Energy	Number (Double)	8
Next Cross section	Number (Double)	8

Cross section

Name	Type	Size
Reaction number	Number (Long)	4
Point number	Number (Long)	4
Energy	Number (Double)	8
Cross section	Number (Double)	8

Group 069[Link]

Name	Type	Size
Reaction number	Number (Long)	4
Group number	Number (Long)	4
Cross section	Number (Double)	8

Group 069_Source

Name	Type	Size
Reaction number	Number (Long)	4
Source ID	Number (Integer)	2
Group number	Number (Long)	4
Cross section	Number (Double)	8

Group 100[Link]

Name	Type	Size
Reaction number	Number (Long)	4
Group number	Number (Long)	4
Cross section	Number (Double)	8

Group 100_Source

Name	Type	Size
Reaction number	Number (Long)	4
Source ID	Number (Integer)	2
Group number	Number (Long)	4
Cross section	Number (Double)	8

Group 172F[Link]

Name	Type	Size
Reaction number	Number (Long)	4
Group number	Number (Long)	4
Cross section	Number (Double)	8

Group 172F_Source

Name	Type	Size
Reaction number	Number (Long)	4
Source ID	Number (Integer)	2
Group number	Number (Long)	4
Cross section	Number (Double)	8

Group 172V[Link]

Name	Type	Size
Reaction number	Number (Long)	4
Group number	Number (Long)	4
Cross section	Number (Double)	8

Group 172W[Link]

Name	Type	Size
Reaction number	Number (Long)	4
Group number	Number (Long)	4
Cross section	Number (Double)	8

Group 172W_Source

Name	Type	Size
Reaction number	Number (Long)	4
Source ID	Number (Integer)	2
Group number	Number (Long)	4
Cross section	Number (Double)	8

Group 175F

Name	Type	Size
Reaction number	Number (Long)	4
Group number	Number (Long)	4
Cross section	Number (Double)	8

Group175F_Source

Name	Type	Size
Reaction number	Number (Long)	4
Source ID	Number (Integer)	2
Group number	Number (Long)	4
Cross section	Number (Double)	8

Group 175V[Link]

Name	Type	Size
Reaction number	Number (Long)	4
Group number	Number (Long)	4
Cross section	Number (Double)	8

Group 175V_Source

Name	Type	Size
Reaction number	Number (Long)	4
Source ID	Number (Integer)	2
Group number	Number (Long)	4
Cross section	Number (Double)	8

Group 211F[Link]

Name	Type	Size
Reaction number	Number (Long)	4
Group number	Number (Long)	4
Cross section	Number (Double)	8

Group 211F_Source

Name	Type	Size
Reaction number	Number (Long)	4
Source ID	Number (Integer)	2
Group number	Number (Long)	4
Cross section	Number (Double)	8

Group 315F[Link]

Name	Type	Size
Reaction number	Number (Long)	4
Group number	Number (Long)	4
Cross section	Number (Double)	8

Group 315F_Source

Name	Type	Size
Reaction number	Number (Long)	4
Source ID	Number (Integer)	2
Group number	Number (Long)	4
Cross section	Number (Double)	8

Group 315V

Name	Type	Size
Reaction number	Number (Long)	4
Group number	Number (Long)	4
Cross section	Number (Double)	8

Group315V_Source

Name	Type	Size
Reaction number	Number (Long)	4
Source ID	Number (Integer)	2
Group number	Number (Long)	4
Cross section	Number (Double)	8

Group 315W

Name	Type	Size
Reaction number	Number (Long)	4
Group number	Number (Long)	4
Cross section	Number (Double)	8

Group 315W_Source

Name	Type	Size
Reaction number	Number (Long)	4
Source ID	Number (Integer)	2
Group number	Number (Long)	4
Cross section	Number (Double)	8

Group 351F[Link]

Name	Type	Size
Reaction number	Number (Long)	4
Group number	Number (Long)	4
Cross section	Number (Double)	8

Group351F_Source

Name	Type	Size
Reaction number	Number (Long)	4
Source ID	Number (Integer)	2
Group number	Number (Long)	4
Cross section	Number (Double)	8

Interpolation

Name	Type	Size
Reaction number	Number (Long)	4
Range number	Number (Integer)	2
Range limit	Number (Long)	4
Interpolation law	Number (Integer)	2

Reaction

Name	Type	Size
Reaction number	Number (Long)	4
Source	Text	50
ZA target	Number (Long)	4
I target	Number (Integer)	2
ZA daughter	Number (Long)	4
I daughter	Number (Integer)	2
Multiplicity	Number (Integer)	2
MT	Number (Integer)	2
QM	Number (Double)	8
QI	Number (Double)	8
LR	Number (Integer)	2
NR	Number (Integer)	2
NP	Number (Long)	4
History	Text	255

Suspect points

Name	Type	Size
Reaction number	Number (Long)	4
Point number	Number (Long)	4
Ratio	Number (Single)	4
Interpolation law	Number (Integer)	2
Treated	Number (Byte)	1

Target

Name	Type	Size
Target number	Number (Long)	4
ZA	Number (Long)	4
I	Number (Integer)	2

Uncertainty

Name	Type	Size
Reaction number	Number (Long)	4
Group number	Number (Long)	4
Energy	Number (Double)	8
DeltaSquared	Number (Double)	8

9. The definition of the EXFOR.mdb *database tables*

Conferences

Name	Type	Size
Code	Text	11
Name	Text	56

CountryCodes

Name	Type	Size
ID	Number(Integer)	2
Name	Text	30
Code	Text	3

Cross section

Name	Type	Size
Full access	Number (Long)	4
Point number	Number (Long)	4
Energy	Number (Double)	8
Delta energy	Number (Double)	8
Cross section	Number (Double)	8
Delta cross section	Number (Double)	8

Evaluated Graphs

Name	Type	Size
ZA	Number (Long)	4
I	Number (Integer)	2
MT	Number (Integer)	2
Status	Number (Integer)	2
Library	Text	50
File name	Text	50

Graphs

Name	Type	Size
ZA	Number (Long)	4
I	Number (Integer)	2
MT	Number (Integer)	2
Status	Number (Integer)	2
File name	Text	50

Journals

Name	Type	Size
Code	Text	10
Name	Text	50

LabCodes

Name	Type	Size
Code	Text	3
ID	Number (Integer)	2
Name	Text	60

Private Cross section

Name	Type	Size
Full access	Number (Long)	4
Point number	Number (Long)	4
Energy	Number (Double)	8
Delta energy	Number (Double)	8
Cross section	Number (Double)	8
Delta cross section	Number (Double)	8

Private Reaction

Name	Type	Size
ZA target	Number (Long)	4
I target	Number (Integer)	2
Full access	Number (Long)	4
FS	Number (Long)	4
MT	Number (Integer)	2
Code	Text	6
NP	Number (Long)	4
Date	Text	4
Type	Text	3
E low	Number (Double)	8
E high	Number (Double)	8
Title	Text	100
Authors	Text	50
Reference	Text	6

Reaction

Name	Type	Size
ZA target	Number (Long)	4
I target	Number (Integer)	2
Full access	Number (Long)	4
FS	Number (Long)	4
MT	Number (Integer)	2
Code	Text	6
NP	Number (Long)	4
UseP	Yes/No	1
Factor E	Number (Double)	8
Factor DE	Number (Double)	8
Factor X	Number (Double)	8
Factor DX	Number (Double)	8

ReacCode

Name	Type	Size
Code	Text	3
MT	Number (Integer)	2
FS	Number (Integer)	2

Reports

Name	Type	Size
Code	Text	11
Name	Text	50

Appendix 2. Practical details

File locations

The locations of the various files used by SAFEPAQ-II are defined in the Settings window (Figure 1). This appendix gives more details of the locations. If several hard disks are available on the computer system, then some of these can be dedicated to SAFEPAQ-II data. If this is not the case then to increase flexibility a special 'hidden folder' can be used. If the folder `Safepaq_2_` is present on the computer (it should be in the root of the 'Source database disk' and the 'SAFEPAQ database disk'), then all the folders defined in the Settings window are assumed to be in this folder. Thus Figure A2.1 shows a typical case with dedicated hard disks, while Figure A2.2 shows a case with the hidden folder.

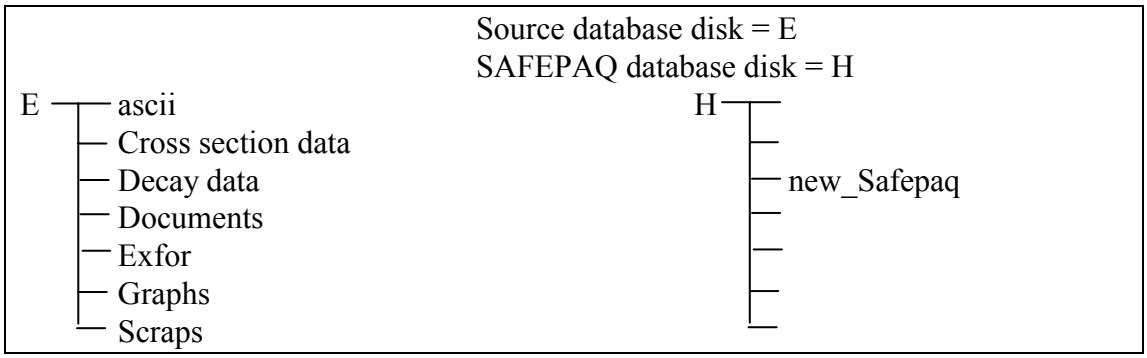


Fig A2.1 Partial disk structure without hidden folder.

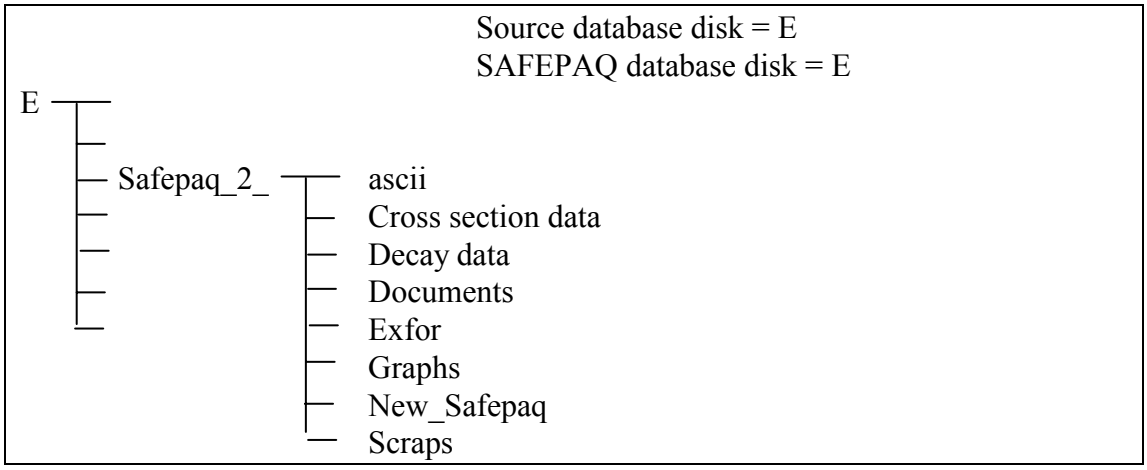


Fig A2.2 Partial disk structure with hidden folder.

In all cases the default location of the safepaq2.exe file is on the 'Base disk' (C) in the folder `Programe Files\safepaq2`.

Linked tables

As the SAFEPAQ-II application has become more sophisticated and the sizes of the EAF projects have increased there are several cases where the databases contain linked tables. This can be a problem when transferring projects between various computers. The reason is that the location of a linked table is specified in terms of the path on the computer where the link was created, if the database is then moved or copied to another disk the link may no longer be valid, causing a crash of SAFEPAQ-II. Although a tool (Linked Table Manager) exists in Access to deal with such problems, it can only be used if the version of the database is the same as the version of Access. Since the SAFEPAQ-II databases all have Access-97 format and increasingly later versions of Access are being used, it is necessary to consider this problem within SAFEPAQ-II.

The linked tables within *compare.mdb* can be dealt with by recreating the database on the new computer, and it is recommended that this be done as soon as SAFEPAQ-II is opened with a new project.

Prior to EAF-2005 the size of *final.mdb* was well below the 1 GB limit that is part of the Access specification. However, with the significant increase in the number of reactions from EAF-2005 this size became a real limitation. In order to overcome this limit most of the tables containing multi-group data (the exception is *Group 175F*) are transferred to the *final_add.mdb* database, and *final.mdb* contains links to the tables in *final_add.mdb*. This change is transparent to the Visual Basic code, but the location of *final_add.mdb* is 'hard-wired' into *final.mdb*. This means that if the specified path does not exist on a computer that both Final databases are moved to, then a crash will occur.

A similar problem occurs for the source databases e.g. *talys5.mdb* under certain circumstances. If the procedure to generate a summary for validation has been carried out for the source database then links are included to *parameter.mdb* of the current project. Again, if the source database is moved to another computer then these links will be incorrect and while the summary can be regenerated, this can be time consuming for large source libraries.

The solution to these problems is to use the 'Linked tables' tool available on the Tools menu of SAFEPAQ-II. This shows the current location held in the link and enables this to be changed to the correct path. Note that when a new project is created the links in the new version of *final.mdb* are automatically changed so as to point to the new version of *final_add.mdb*.

Another problem with links also has to be avoided when a new EAF project is created. This arises because when the files are copied to a new folder, the new *final.mdb* still contained links to the original *final_add.mdb*. When the data in the new *final.mdb* were removed, what actually happened for the group data was that the original *final_add.mdb* was cleared. This problem has been corrected and the links are automatically updated when the new project is created.

x4s file format

Private EXFOR data are held in an x4s file. The format of the file is illustrated below.

```
2    9  2
GEO65
Energy (MeV)  Xsect (mb)   D-Xsect (mb)
 1.3940E+01   1.1000E-01   2.0000E-02
 1.4500E+01   2.1000E-01   4.0000E-02
 1.4920E+01   2.1000E+00   4.0000E-01
 1.5350E+01   4.5000E+00   6.0000E-01
 1.5890E+01   5.4000E+00   1.0000E+00
 1.6500E+01   1.3000E+01   2.0000E+00
 1.7060E+01   2.6000E+01   0.0000E+00
 1.7490E+01   2.6000E+01   4.0000E+00
 1.7980E+01   3.8000E+01   5.0000E+00
  3    1  2
ITJ73
Energy (MeV)  Xsect (mb)   D-Xsect (mb)
 1.4000E+01   1.3000E-01   5.0000E-02
```

Line 1 contains the number of the data set (any unique value can be used) in positions 1-3, the number of points in the data set in positions 5-9 and the final state identifier (0, 1, 2, 99 or blank = 99 can be used) in position 10-11.

Line 2 contains the data set identifier (XXXnn format) in positions 1-5.

Line 3 contains the data headers, note that units must be given, these can only be ‘eV’, ‘MeV’, ‘b’ or ‘mb’. The data can be in two columns (Energy and Xsect) or three columns (Energy, Xsect and D-Xsect).

Following lines show the data points is standard scientific notation.

The next data set then follows with no blank line separating the data.

XY table file format

One of the options for the format of the source data files is ‘XY table’, see the Library options window (Figure 23). The format of the file is illustrated below.

```
 18039  0
   102 99
     2
    49
2.00000E+00 3.84000E+01
4.60000E+00 1.75000E+01
1.00000E+01 8.30000E+00
1.50000E+01 5.58000E+00
2.20000E+01 3.84000E+00
```

Line 1 contains the ZA identifier of the target in positions 1-6, and the initial state of the target (0, 1, 2) in postion 9.

Line 2 contains the reaction MT number in positions 4-6 and the daughter final state (0, 1, 2, 99) in positions 8-9.

Line 3 contains the interpolation law (only one law is possible) in position 6.

Line 4 contains the number of data points in positions 3-6.

Following lines show the data points (energy, cross section) in standard scientific notation. The data must be in the format shown (5 decimal places) starting in columns 1 and 13.

Scrap file format

Data scraps are held in a very similar file format to the 'XY table' however Lines 1 and 2 are not present.

Appendix 3. Multi-group cross sections

Introduction

Calculations of multi-group cross sections are made exactly in SAFEPAQ-II, *i.e.* by summing the contributions made by all pairs of data points in a particular group. The data points and the interpolation law define exactly the form of the cross section in that range and by using one of a small number of weighting functions the contribution can be analytically evaluated. Note that it is assumed that the weighting function cannot change between any two points.

For a particular energy group the definition of group cross section is given in equation (1), where $\phi(E)$ is the weighting function in the group, $\sigma(E)$ is the cross section and ϕ_g is the value of the weighting function integrated over the group.

$$\sigma_g = \frac{1}{\phi_g}\int_g \phi(E)\sigma(E)dE \quad \text{.....(1)}$$

If there are *n* data points in the group, then it is necessary to add the two additional points that lie on the upper and lower boundaries. The cross section values for these are obtained by interpolation.

Thus the value of the multi-group cross section will be given by equation (2), where E_i is the energy of the *i*th point.

$$\sigma_g = \frac{1}{\phi_g}\sum_{i=0}^{n+1}\int_{E_i}^{E_{i+1}} \phi(E)\sigma(E)dE \quad \text{.....(2)}$$

By the use of one of the five standard interpolation laws, $\sigma(E)$ is expressible as an analytical formula, and $\phi(E)$ is one of five standard formulae. The five standard forms of weighting function are shown in equations (3) - (7).

$$\phi(E) = C \quad \{\text{Flat weighting}\} \text{.....(3)}$$

$$\phi(E) = C/E \quad \{\text{1/E weighting}\} \text{.....(4)}$$

$$\phi(E) = CE\ \exp(-E/kT) \quad \{\text{Maxwellian thermal weighting}\} \text{.....(5)}$$

$$\phi(E) = C\sqrt{E}\ \exp(-E/T_f) \quad \{\text{Fission spectrum weighting}\} \text{.....(6)}$$

$$\phi(E) = C\exp\left(-5/kT_f(\sqrt{E} - \sqrt{E_f})\right) \quad \{\text{Velocity exponential fusion weighting}\} \text{.(7)}$$

In these equations, C is a constant, kT = 0.0253 eV, kT_f = 1.4 MeV (in (6)), kT_f = 0.025 MeV (in (7)) and E_f = 14.07 MeV.

The problem of calculating the 25 expressions resulting from using these weighting functions and interpolation laws yields simple analytical expressions in most cases. However, for the fission spectrum weighting some of the analytical expressions are very complicated (involving Error and Hypergeometric functions) and it is be preferable to replace equation (6) by a quadratic function that fits (6) extremely well.

Interpolation laws

Expressions for the form of the cross section are given in terms of the energies (E_1 and E_2) and cross sections (σ_1 and σ_2).

Law 1, constant

$$\sigma(E) = \sigma_1 \text{.....(8)}$$

Law 2, linear-linear

$$\sigma(E) = \sigma_1 + \frac{\sigma_2 - \sigma_1}{E_2 - E_1}(E - E_1) = A + BE \text{.....(9)}$$

$$\Rightarrow A = \frac{\sigma_1 E_2 - \sigma_2 E_1}{E_2 - E_1}; B = \frac{\sigma_2 - \sigma_1}{E_2 - E_1} \quad \text{.....(10)}$$

Law 3, log-linear

$$\sigma(E) = \sigma_1 + \frac{\sigma_2 - \sigma_1}{\ln(E_2) - \ln(E_1)}\big(\ln(E) - \ln(E_1)\big) = A + B\ln(E) \quad \text{...(11)}$$

$$\Rightarrow A = \frac{\sigma_1 \ln(E_2) - \sigma_2 \ln(E_1)}{\ln(E_2) - \ln(E_1)}; B = \frac{\sigma_2 - \sigma_1}{\ln(E_2) - \ln(E_1)} \quad \text{.....(12)}$$

Law 4, linear-log

$$\ln(\sigma(E)) = \ln(\sigma_1) + \frac{\ln(\sigma_2) - \ln(\sigma_1)}{E_2 - E_1}\big(E - E_1\big) = A + BE \quad \text{.....(13)}$$

$$\Rightarrow \sigma(E) = e^A e^{BE} \quad \text{.....(14)}$$

$$\Rightarrow A = \frac{\ln(\sigma_1)E_2 - \ln(\sigma_2)E_1}{E_2 - E_1}; B = \frac{\ln(\sigma_2) - \ln(\sigma_1)}{E_2 - E_1} \quad \text{.....(15)}$$

Law 5, log-log

$$\ln(\sigma(E)) = \ln(\sigma_1) + \frac{\ln(\sigma_2) - \ln(\sigma_1)}{\ln(E_2) - \ln(E_1)}\big(\ln(E) - \ln(E_1)\big) = A + B\ln(E) \quad (16)$$

$$\Rightarrow \sigma(E) = e^A E^B \quad \text{.....(17)}$$

$$\Rightarrow A = \frac{\ln(\sigma_1)\ln(E_2) - \ln(\sigma_2)\ln(E_1)}{\ln(E_2) - \ln(E_1)}; B = \frac{\ln(\sigma_2) - \ln(\sigma_1)}{\ln(E_2) - \ln(E_1)} \quad \text{.....(18)}$$

Flat weighting

Using equation (3) for the weighting and each interpolation law in term yields the following expressions for the multi-group cross section integral $J = \int \phi(E)\sigma(E)dE$.

Law 1

$$J(E_1, E_2) = C\sigma_1 \int_{E_1}^{E_2} dE = C\sigma_1(E_2 - E_1) \quad \text{.....(19)}$$

Law 2

$$\begin{aligned} J(E_1, E_2) &= C\int_{E_1}^{E_2} (A + BE)dE = CA(E_2 - E_1) + \tfrac{1}{2}CB(E_2^2 - E_1^2) \\ &= \tfrac{1}{2}C(\sigma_1 + \sigma_2)(E_2 - E_1) \end{aligned} \quad \text{..(20)}$$

Law 3

$$\begin{aligned} J(E_1, E_2) &= C\int_{E_1}^{E_2} (A + B\ln(E))dE = CA(E_2 - E_1) + CB\left[E\ln(E) - E\right]_{E_1}^{E_2} \\ &= C(A - B)(E_2 - E_1) + CB(E_2\ln(E_2) - E_1\ln(E_1)) \end{aligned} \quad (21)$$

Law 4

$$J(E_1,E_2) = Ce^A \int_{E_1}^{E_2} e^{BE}dE = \frac{C}{B}e^A\left[e^{BE}\right]_{E_1}^{E_2}$$
$$= \frac{C}{B}e^A\left(e^{BE_2} - e^{BE_1}\right) \text{for } B \neq 0 \quad \text{.....(22)}$$
$$= Ce^A(E_2 - E_1) \text{ for } B = 0$$

Law 5

$$J(E_1,E_2) = Ce^A \int_{E_1}^{E_2} E^B dE = \frac{Ce^A}{(B+1)}\left[E^{B+1}\right]_{E_1}^{E_2}$$
$$= \frac{Ce^A}{(B+1)}\left(E_2^{B+1} - E_1^{B+1}\right) \text{for } B \neq 0 \text{ and } B \neq -1 \quad \text{.....(23)}$$
$$= Ce^A(E_2 - E_1) \text{ for } B = 0$$
$$= Ce^A \ln(E_2/E_1) \text{ for } B = -1$$

1/E weighting

Using equation (4) for the weighting and each interpolation law in term yields the following expressions for the multi-group cross section *J*. Note that these are the same formulae as used in the calculation of the resonance integral.

Law 1

$$J(E_1,E_2) = C\sigma_1 \int_{E_1}^{E_2} \frac{dE}{E} = C\sigma_1 \ln(\frac{E_2}{E_1}) \quad \text{.....(24)}$$

Law 2

$$J(E_1,E_2) = C\int_{E_1}^{E_2} \frac{(A+BE)}{E}dE = CA\ln(\frac{E_2}{E_1}) + CB(E_2 - E_1)$$
$$= CA\ln(\frac{E_2}{E_1}) + C(\sigma_2 - \sigma_1) \quad (25)$$

Law 3

Using the standard integral (A2):

$$J(E_1,E_2) = C\int_{E_1}^{E_2} \frac{(A+B\ln(E))}{E}dE = CA\ln(\frac{E_2}{E_1}) + \tfrac{1}{2}CB\left[(\ln(E))^2\right]_{E_1}^{E_2}$$
$$= CA(\ln(E_2) - \ln(E_1)) + \tfrac{1}{2}CB(\ln(E_2) - \ln(E_1))(\ln(E_2) + \ln(E_1)) \quad (26)$$
$$= \tfrac{1}{2}C(\sigma_1 + \sigma_2)\ln(\frac{E_2}{E_1})$$

Law 4

$$J(E_1,E_2) = Ce^A \int_{E_1}^{E_2} \frac{e^{BE}}{E} dE \quad \text{.....(27)}$$

Using the standard result, shown in equation (A3), and defining $I_n(E_1,E_2,\alpha)$ by equation (28) the final expression is given in (29).

$$I_n(E_1,E_2,\alpha) = \int_{E_1}^{E_2} E^n e^{\alpha E} dE \quad \text{.....(28)}$$

$$J(E_1,E_2) = Ce^A I_{-1}(E_1,E_2,B) \quad \text{.....(29)}$$

Law 5

$$\begin{aligned} J(E_1,E_2) &= Ce^A \int_{E_1}^{E_2} E^{B-1} dE = \frac{Ce^A}{B}\left[E^B\right]_{E_1}^{E_2} \\ &= \frac{Ce^A}{B}\left(E_2^B - E_1^B\right) \text{for } B \neq 0 \text{ and } B \neq 1 \\ &= Ce^A (E_2 - E_1) \text{ for } B = 1 \\ &= Ce^A \ln(E_2/E_1) \text{ for } B = 0 \end{aligned} \quad \text{.....(30)}$$

Maxwellian thermal weighting

Using equation (5) for the weighting and each interpolation law in term yields the following expressions for the multi-group cross section integral *J*.

Law 1

$$J(E_1,E_2) = C\sigma_1 \int_{E_1}^{E_2} E \exp(-E/kT) dE \quad \text{.....(31)}$$

Using the standard result, shown in equation (A1), and using $I_n(E_1,E_2,\alpha)$ defined by equation (28), the final expression is given in (32).

$$J(E_1,E_2) = C\sigma_1 I_1(E_1,E_2,-1/kT) \quad \text{.....(32)}$$

Law 2

$$\begin{aligned} J(E_1,E_2) &= C\int_{E_1}^{E_2} (A+BE)E\exp(-E/kT)dE \\ &= CAI_1(E_1,E_2,-1/kT) + CBI_2(E_1,E_2,-1/kT) \end{aligned} \quad \text{.....(33)}$$

Law 3

$$J(E_1,E_2) = C\int_{E_1}^{E_2}(A+B\ln(E))E\exp(-E/kT)\,dE$$
$$= CAI_1(E_1,E_2,-1/kT) + CBk^2T^2I_{-1}(E_1,E_2,-1/kT) - \quad \text{....(34)}$$
$$CBk^2T^2\left[\exp(-E/kT)\left(\frac{(E+kT)\ln(E)}{kT}+1\right)\right]_{E_1}^{E_2}$$

Law 4

$$J(E_1,E_2) = Ce^A\int_{E_1}^{E_2}Ee^{BE}\exp(-E/kT)dE = Ce^A\int_{E_1}^{E_2}E\exp\left(\frac{-E(1-BkT)}{kT}\right)dE \quad .(35)$$

Defining a new variable ε such that $\varepsilon = (1-kTB)E$ means that (35) can be written as (36).

$$J(E_1,E_2) = \frac{Ce^A}{(1-kTB)^2}\int_{(1-kTB)E_1}^{(1-kTB)E_2}\varepsilon\exp(-\varepsilon/kT)d\varepsilon$$
$$= \frac{Ce^A}{(1-kTB)^2}I_1\left((1-kTB)E_1,(1-kTB)E_2,-1/kT\right), \text{ where } B\neq 1/kT \quad \text{.....(36)}$$
$$= \frac{1}{2}Ce^A(E_2^2-E_1^2), \text{ where } B = 1/kT$$

Law 5

$$J(E_1,E_2) = Ce^A\int_{E_1}^{E_2}E^{B+1}\exp(-E/kT)dE \quad \text{.....(37)}$$

Note that in equation (37) B is not generally an integer, and the solution for non-integer B involves incomplete gamma functions. The solution for integral B is given in equation (38), for the general case the solution using gamma functions is shown in equation (39).

$$J(E_1,E_2) = Ce^AI_{B+1}(E_1,E_2,-1/kT) \quad \text{.....(38)}$$

Equation (37) can be written as equation (39) using equation (A13).

$$J(E_1,E_2) = Ce^A(kT)^{B+2}\Gamma(B+2)\left[P(B+2,E_2/kT)-P(B+2,E_1/kT)\right] \text{ with } B>-2 \quad (39)$$

Equation (39) is only valid for $B > -2$, in order to extend the range to more negative vales of B, equation (37) can be integrated by parts. $K_1(E_1,E_2)$ is defined by equation (40) and $F_n(E_1,E_2)$ by equation (41).

$$J(E_1,E_2) = Ce^AK_1(E_1,E_2) \quad \text{.....(40)}$$

$$F_n(E_1,E_2)=\frac{1}{(B+n)}\left[E_2^{B+n}\exp(-E_2/kT)-E_1^{B+n}\exp(-E_1/kT)\right] \quad .....(41)$$

Then K_1 can be written in several forms as shown in equations (42) – (44) following integration by parts.

$$K_1=F_2+\frac{K_2}{kT(B+2)} \quad .....(42)$$

$$K_1=F_2+\frac{F_3}{kT(B+2)}+\frac{K_3}{(kT)^2(B+2)(B+3)} \quad .....(43)$$

$$K_1=F_2+\frac{F_3}{kT(B+2)}+\frac{F_4}{(kT)^2(B+2)(B+3)}+\frac{K_4}{(kT)^3(B+2)(B+3)(B+4)} \quad (44)$$

K_n can be written in terms of gamma functions in a similar fashion to equation (39) as shown in equation (45).

$$K_n(E_1,E_2)=(kT)^{B+n+1}\Gamma(B+n+1)\left[P(B+n+1,E_2/kT)-P(B+n+1,E_1/kT)\right] \text{ with } B>-(1+n)$$
$$.....(45)$$

For more negative values of B, a quadratic fit as described in the following section is used.

Fission spectrum weighting

Using equation (6) for the weighting leads to extremely complicated integrals. Over the energy range of interest it is possible to very accurately fit the weighting function to a simple quadratic function shown in (46). The constants are found by fitting to the original function. Using this and each interpolation law in term yields the following expressions for the multi-group cross section integral *J*.

$$\phi(E)=\alpha+\beta E+\gamma E^2 \quad .....(46)$$

Law 1

$$\begin{aligned}J(E_1,E_2)&=\sigma_1\int_{E_1}^{E_2}(\alpha+\beta E+\gamma E^2)dE\\&=\sigma_1\left[\alpha E+\tfrac{1}{2}\beta E^2+\tfrac{1}{3}\gamma E^3\right]_{E_1}^{E_2}\\&=\sigma_1\left(\alpha(E_2-E_1)+\tfrac{1}{2}\beta(E_2^2-E_1^2)+\tfrac{1}{3}\gamma(E_2^3-E_1^3)\right)\end{aligned} \quad (47)$$

Law 2

$$J(E_1,E_2)=\int_{E_1}^{E_2}(A+BE)(\alpha+\beta E+\gamma E^2)dE$$
$$=\int_{E_1}^{E_2}\alpha A+\beta AE+\gamma AE^2+\alpha BE+\beta BE^2+\gamma BE^3 dE$$
$$=\left[\alpha AE+\tfrac{1}{2}(\beta A+\alpha B)E^2+\tfrac{1}{3}(\gamma A+\beta B)E^3+\tfrac{1}{4}\gamma BE^4\right]_{E_1}^{E_2}$$
$$=\left(\alpha A(E_2-E_1)+\tfrac{1}{2}(\beta A+\alpha B)(E_2^2-E_1^2)+\tfrac{1}{3}(\gamma A+\beta B)(E_2^3-E_1^3)+\tfrac{1}{4}\gamma B(E_2^4-E_1^4)\right)$$
.....(48)

Law 3

$$J(E_1,E_2)=\int_{E_1}^{E_2}(A+B\ln(E))(\alpha+\beta E+\gamma E^2)dE$$
$$=\int_{E_1}^{E_2}\alpha A+\beta AE+\gamma AE^2+\alpha B\ln(E)+\beta BE\ln(E)+\gamma BE^2\ln(E)dE$$
..(49)

Using the standard integrals shown in (A6)-(A8) this integral can be evaluated as shown in equation (50).

$$J(E_1,E_2)=\left[\begin{array}{l}\alpha AE+\tfrac{1}{2}\beta AE^2+\tfrac{1}{3}\gamma AE^3+\alpha BE\ln(E)-\alpha BE+\tfrac{1}{2}\beta BE^2\ln(E)-\tfrac{1}{4}\beta BE^2\ldots\\ \ldots+\tfrac{1}{3}\gamma BE^3\ln(E)-\tfrac{1}{9}\gamma BE^3\end{array}\right]_{E_1}^{E_2}$$
$$=\left[\alpha(A-B)E+\tfrac{1}{4}\beta(2A-B)E^2+\tfrac{1}{9}\gamma(3A-B)E^3+\tfrac{1}{6}B(6\alpha+3\beta E+2\gamma E^2)E\ln(E)\right]_{E_1}^{E_2}$$
.....(50)

Law 4

$$J(E_1,E_2)=e^A\int_{E_1}^{E_2}e^{BE}(\alpha+\beta E+\gamma E^2)dE$$
$$=\frac{e^A}{B}\left[(\alpha+\beta E+\gamma E^2)e^{BE}\right]_{E_1}^{E_2}-\frac{e^A}{B}\int_{E_1}^{E_2}e^{BE}(\beta+2\gamma E)dE$$
$$=\frac{e^A}{B}\left[(\alpha+\beta E+\gamma E^2)e^{BE}-(\beta+2\gamma E)\frac{e^{BE}}{B}\right]_{E_1}^{E_2}+\frac{e^A}{B^2}\int_{E_1}^{E_2}e^{BE}2\gamma dE$$ ...(51)
$$=\frac{e^A}{B}\left[(\alpha+\beta E+\gamma E^2)e^{BE}-(\beta+2\gamma E)\frac{e^{BE}}{B}+2\gamma\frac{e^{BE}}{B^2}\right]_{E_1}^{E_2}$$
$$=\frac{e^A}{B^3}\left[e^{BE}(\alpha B^2-\beta B+2\gamma+B(\beta B-2\gamma)E+\gamma B^2E^2)\right]_{E_1}^{E_2}$$

Law 5

$$J(E_1,E_2)=e^A\int_{E_1}^{E_2}E^B(\alpha+\beta E+\gamma E^2)dE=e^A\int_{E_1}^{E_2}\alpha E^B+\beta E^{B+1}+\gamma E^{B+2}dE$$ .....(52)

Equation (52) can be solved trivially except for three values of B = -1, -2, -3. In these cases a log term is introduced.

$$J(E_1,E_2) = e^A\left[\frac{\alpha E^{B+1}}{B+1}+\frac{\beta E^{B+2}}{B+2}+\frac{\gamma E^{B+3}}{B+3}\right]_{E_1}^{E_2}, \text{ where } B \neq \{-1,-2,-3\}$$
$$= e^A\left[\alpha\ln(E)+\frac{\beta E^{B+2}}{B+2}+\frac{\gamma E^{B+3}}{B+3}\right]_{E_1}^{E_2}, \text{ where } B=-1$$
$$= e^A\left[\frac{\alpha E^{B+1}}{B+1}+\beta\ln(E)+\frac{\gamma E^{B+3}}{B+3}\right]_{E_1}^{E_2}, \text{ where } B=-2 \quad \text{.....(53)}$$
$$= e^A\left[\frac{\alpha E^{B+1}}{B+1}+\frac{\beta E^{B+2}}{B+2}+\gamma\ln(E)\right]_{E_1}^{E_2}, \text{ where } B=-3$$

Velocity exponential fusion

Equation (7) can be rewritten in a simpler form as shown in equation (54), where $g = 5\sqrt{E_f}\,/kT_f$ and $a = -5/kT_f$. Using equation (54) for the weighting and each interpolation law in term yields the following expressions for the multi-group cross section integral *J*.

$$\phi(E) = Cg\,\exp\left(aE^{1/2}\right) \quad \text{.....(54)}$$

Law 1

$$J(E_1,E_2) = Cg\,\sigma_1\int_{E_1}^{E_2}\exp(\,aE^{1/2})dE \quad \text{.....(55)}$$

By changing the variable, $E = z^2$, equation (55) can be written as equation (56).

$$J(E_1,E_2) = 2Cg\,\sigma_1\int_{\sqrt{E_1}}^{\sqrt{E_2}} z\exp(\,az)dz \quad \text{.....(56)}$$

Using the integral shown in equation (28), this integral can be evaluated as shown in equation (57).

$$J(E_1,E_2) = 2Cg\,\sigma_1 I_1(E_1^{1/2},E_2^{1/2},-5/kT_f) \quad \text{.....(57)}$$

Law 2

$$J(E_1,E_2) = Cg\int_{E_1}^{E_2}(A+BE)\exp(\,aE^{1/2})dE$$
$$= 2CgAI_{\,1}(E_1^{1/2},E_2^{1/2},-5/kT_f) + CgB\int_{E_1}^{E_2}E\exp(\,aE^{1/2})dE \quad \text{....(58)}$$

Changing the variable as in Law 1 enables the second integral to be written in standard form yielding equation (59).

$$J(E_1,E_2) = 2CgAI_{\,1}(E_1^{1/2},E_2^{1/2},-5/kT_f) + 2CgBI_{\,3}(E_1^{1/2},E_2^{1/2},-5/kT_f) \quad \text{.(59)}$$

Law 3

$$J(E_1,E_2) = Cg\int_{E_1}^{E_2}(A + B\ln(E))\exp(aE^{1/2})dE$$
$$= 2CgAI_{1}(E_1^{1/2},E_2^{1/2},-5/kT_f) + CgB\int_{E_1}^{E_2}\ln(E)\exp(aE^{1/2})dE \quad (60)$$

Defining the integral in the second term in equation (60) as shown in equation (61).

$$K(E_1,E_2) = \int_{E_1}^{E_2}\ln(E)\exp(aE^{1/2})dE \quad \text{.....(61)}$$

Changing the variable as in Law 1, carrying out integration by parts and noting that $\frac{d}{dz}\ln(z^2) = \frac{2}{z}$ enables equation (61) to be written as equation (62).

$$K = \frac{2}{a}\ln(z^2)\left(ze^{az} - \frac{1}{a}e^{az}\right) - \frac{4}{a^2}e^{az} + \frac{4}{a^2}\int\frac{e^{az}}{z}dz \quad \text{.....(62)}$$

Changing the variable back to E, equation (62) can be written in standard form in equation (63).

$$K(E_1,E_2) = 2\left[\exp(aE^{1/2})\left(\ln(E)\left(\frac{E^{1/2}}{a} - \frac{1}{a^2}\right) - \frac{2}{a^2}\right)\right]_{E_1}^{E_2} + \frac{4}{a^2}I_{-1}(E_1^{1/2},E_2^{1/2},a) \quad (63)$$

Law 4

$$J(E_1,E_2) = Cge^{A}\int_{E_1}^{E_2}e^{BE}\exp(aE^{1/2})dE = Ce^{A}\int_{E_1}^{E_2}\exp\left(BE + aE^{1/2}\right)dE \quad (64)$$

Equation (64) can be solved in terms of Error functions (a < 0, but B can be either positive or negative meaning that the Imaginary error function would be required). It would be more practical to use a quadratic fit to the weighting spectrum this yields equation (65), which has been solved in equation (51) in section 6.4.

$$J(E_1,E_2) = e^{A}\int_{E_1}^{E_2}e^{BE}(\alpha + \beta E + \gamma E^2)dE \quad \text{.....(65)}$$

Law 5

$$J(E_1,E_2) = Cge^{A}\int_{E_1}^{E_2}E^{B}\exp(aE^{1/2})dE \quad \text{.....(66)}$$

Changing the variable as in section 7.1 enables equation (66) to be written as equation (67).

$$J(E_1,E_2) = 2Cge^{A}\int_{\sqrt{E_1}}^{\sqrt{E_2}}z^{2B+1}e^{az}dz \quad \text{.....(67)}$$

If (2*B*+1) is an integer then equation (67) can be solved by equation (68), otherwise it is the same form as equation (37) which was solved using gamma functions. The solution is given in equation (69).

$$J(E_1,E_2) = 2Cge^{A} I_{2B+1}(E_1^{1/2}, E_2^{1/2}, -5/kT_f) \quad \text{.....(68)}$$

$$J(E_1,E_2) = 2Cge^{A}\left(\frac{kT_f}{5}\right)^{2B+2}\Gamma(2B+2)\left[P\left(2B+2,\frac{5\sqrt{E_2}}{kT_f}\right)-P\left(2B+2,\frac{5\sqrt{E_1}}{kT_f}\right)\right] \text{ with } B>-1$$

.....(69)

Equation (69) is only valid for $B > -1$, in order to extend the range to more negative vales of *B*, equation (67) can be integrated by parts. $K_1(E_1,E_2)$ is defined by equation (70) and $F_n(E_1,E_2)$ by equation (71).

$$J(E_1,E_2) = 2Ce^{A} K_1(E_1,E_2) \quad \text{.....(70)}$$

$$F_n(E_1,E_2) = \frac{1}{(2B+n)}\left[\sqrt{E_2}^{2B+n}\exp(-5\sqrt{E_2}/kT_f) - \sqrt{E_1}^{2B+n}\exp(-5\sqrt{E_1}/kT_f)\right] \text{ ..(71)}$$

Then K_1 can be written in several forms as shown in equations (72) – (74) following integration by parts.

$$K_1 = F_2 + \frac{5K_2}{kT_f(2B+2)} \quad \text{.....(72)}$$

$$K_1 = F_2 + \frac{5F_3}{kT_f(2B+2)} + \frac{5^2K_3}{(kT_f)^2(2B+2)(2B+3)} \quad \text{.....(73)}$$

$$K_1 = F_2 + \frac{5F_3}{kT_f(2B+2)} + \frac{5^2F_4}{(kT_f)^2(2B+2)(2B+3)} + \frac{5^3K_4}{(kT_f)^3(2B+2)(2B+3)(2B+4)}$$

.....(74)

K_n can be written in terms of gamma functions in a similar fashion to equation (69) as shown in equation (75).

$$K_n(E_1,E_2) = \left(\frac{kT_f}{5}\right)^{2B+n+1}\Gamma(2B+n+1)\left[P\left(2B+n+1,\frac{5\sqrt{E_2}}{kT_f}\right)-P\left(2B+n+1,\frac{5\sqrt{E_1}}{kT_f}\right)\right]$$

with $B > -(1+n)/2$

.....(75)

For more negative values of B, a quadratic fit as described in the fission spectrum weighting section is used.

Summary

A summary of the method of solution in each of the 25 cases is given in the following table. Note that 'Simple' indicates an algebraic function of E_1, E_2, σ_1 and σ_2, 'Quadratic fit' indicates that due to the complexity of the solution a quadratic fit to the weighting spectrum over the energy range has been adopted and '$\sim I_n$ indicates that an algebraic expression and the standard integral shown in equation (28) has been used. 'Gamma fun' indicates that an incomplete gamma function has been used.

Weighting→ Law ↓	Flat	1/E	Maxwellian thermal	Fission spectrum	Velocity exp. fusion
1 - constant	Simple	Simple	$\sim I_1$	Quadratic fit	$\sim I_1$
2 - lin/lin	Simple	Simple	$\sim I_1 + I_2$	Quadratic fit	$\sim I_1 + I_3$
3 - log E/lin σ	Simple	Simple	$\sim I_1 + I_{-1}$	Quadratic fit	$\sim I_1 + I_{-1}$
4 - lin E/ log σ	Simple	$\sim I_{-1}$	$\sim I_1$	Quadratic fit	Quadratic fit
5 - log/log	Simple	Simple	Gamma fun	Quadratic fit	Gamma fun

Annex: Standard integrals

See reference [1] for all except (A13), which is taken from [2]:

$$\int x^m e^{ax}\,dx = e^{ax}\sum_{r=0}^{m}(-1)^r\frac{m!\,x^{m-r}}{(m-r)!\,a^{r+1}} \quad \text{.....(A1)}$$

$$\int \frac{\ln(x)}{x}\,dx = \tfrac{1}{2}(\ln(x))^2 \quad \text{.....(A2)}$$

$$\int \frac{e^{ax}}{x}\,dx = \ln(x) + \sum_{i=1}^{\infty}\frac{(ax)^i}{ii!} \quad \text{.....(A3)}$$

$$\int \ln(x)e^{ax}\,dx = \frac{1}{a}\left(\ln(x)(e^{ax}-1) - \sum_{i=1}^{\infty}\frac{(ax)^i}{ii!}\right) \quad \text{.....(A4)}$$

$$\int x\ln(x)e^{ax}\,dx = \frac{e^{ax}}{a^2}\left((ax-1)\ln(x)-1\right) + \frac{1}{a^2}\left(\ln(x) + \sum_{i=1}^{\infty}\frac{(ax)^i}{ii!}\right) \quad \text{.(A5)}$$

$$\int \ln(x)\,dx = x\ln(x) - x \quad \text{.....(A6)}$$

$$\int x\ln(x)\,dx = \tfrac{1}{2}x^2\ln(x) - \tfrac{1}{4}x^2 \quad \text{.....(A7)}$$

$$\int x^2\ln(x)\,dx = \tfrac{1}{3}x^3\ln(x) - \tfrac{1}{9}x^3 \quad \text{.....(A8)}$$

Explicit formulae for the standard integral $I_n(E_1,E_2,\alpha)$ defined in equation (28) are given for n = -1, 1, 2, 3.

$$I_1(E_1,E_2,\alpha) = \frac{1}{\alpha^2}\left[(\alpha E_2 - 1)e^{\alpha E_2} - (\alpha E_1 - 1)e^{\alpha E_1}\right] \quad \text{.....(A9)}$$

$$I_2(E_1,E_2,\alpha)=\frac{1}{\alpha^3}\left[(\alpha^2E_2^2-2\alpha E_2+2)e^{\alpha E_2}-(\alpha^2E_1^2-2\alpha E_1+2)e^{\alpha E_1}\right] \quad \text{(A10)}$$

$$I_3(E_1,E_2,\alpha)=\frac{1}{\alpha^4}\left[(\alpha^3E_2^3-3\alpha^2E_2^2+6\alpha E_2-6)e^{\alpha E_2}-(\alpha^3E_1^3-3\alpha^2E_1^2+6\alpha E_1-6)e^{\alpha E_1}\right] \quad \text{(A11)}$$

$$I_{-1}(E_1,E_2,\alpha)=\ln(E_2/E_1)+\sum_{i=1}^{\infty}\frac{\alpha^i(E_2^i-E_1^i)}{ii!} \quad \text{(A12)}$$

$$P(a,x)=\frac{1}{\Gamma(a)}\int_0^x t^{a-1}e^{-t}dt \quad a>0 \quad \text{(A13)}$$

References

[1] CRC Handbook of Chemistry and Physics, Editor R. C. Weast, 68th Edition, 1998.

[2] Numerical Recipes in Fortran, 2nd Edition, W.H. Press, S.A. Teukolsky, W.T. Vetterling and B.P. Flannery, Cambridge University Press, 1992.

Appendix 4. Branching ratios

An inconsistent definition of the branching ratio was used in SYMPAL. This was corrected in later stages of the processing. The following description shows the definition used in SAFEPAQ-II.

If there is only a single isomeric state then the branching ratio is defined by equation (1).

$$b_m = \frac{\sigma_m}{\sigma_m + \sigma_g} \quad \text{.....(1)}$$

This branching ratio can be calculated by systematics.

If there is a second isomeric state then the branching ratio for this state (on the assumption that it is the only one), is given by equation (2).

$$b_n = \frac{\sigma_n}{\sigma_n + \sigma_g} \quad \text{.....(2)}$$

In SYMPAL, and in early versions of SAFEPAQ-II an incorrect assumption about how to form b_g from the other two b's had been made. It was assumed that equation (3) should be used.

$$b_g = 1 - b_m - b_n \quad \text{.....(3)}$$

It can be easily seen that if b_m and b_n are > 0.5 then b_g will be negative. Errors like this were discovered in early versions of SAFEPAQ-II by the presence of negative cross sections.

The correct way to proceed is to assume that the ratios σ_m/σ_g and σ_n/σ_g remain constant irrespective of whether the number of final states is 2 or 3. The values of these ratios are given in equations (4) and (5).

$$\frac{\sigma_m}{\sigma_g} = \frac{b_m}{(1-b_m)} \quad \text{.....(4)}$$

$$\frac{\sigma_n}{\sigma_g} = \frac{b_n}{(1-b_n)} \quad \text{.....(5)}$$

If σ_T is the sum of the three final states, then the ith 3-state branching ratio is given by equation (6).

$$\tilde{b}_i = \frac{\sigma_i}{\sigma_T} \quad \text{.....(6)}$$

Thus for the 1st isomeric state, equation (6) can be rewritten in equation (7).

$$\tilde{b}_m = \frac{\sigma_m}{\sigma_g + \sigma_m + \sigma_n} = \frac{\sigma_m/\sigma_g}{1 + \sigma_m/\sigma_g + \sigma_n/\sigma_g} = \frac{b_m(1-b_n)}{1-b_m b_n} \quad \text{.....(7)}$$

Similarly the other two ratios are given in equations (8) and (9).

$$\tilde{b}_n = \frac{b_n(1-b_m)}{1-b_m b_n} \quad \text{.....(8)}$$

$$\tilde{b}_g = \frac{(1-b_n)(1-b_m)}{1-b_m b_n} \quad \text{.....(9)}$$

Note that the sum of equations (7), (8) and (9) is 1 as required.

Thus equation (3) must be replaced by equation (10).

$$\tilde{b}_g = 1 - \tilde{b}_m - \tilde{b}_n \quad \text{.....(10)}$$

Appendix 5. Single Resonance Approximation

If the thermal cross section is large then it is a physically reasonable approximation to assume that the thermal cross section (and to some extent the resonance integral) are determined by a single strong s-wave resonance. The single level Breit-Wigner (SLBW) formula can be written as shown in equation (1),

$$\sigma = \frac{\pi g_J}{k^2} \frac{\Gamma_n \Gamma_\gamma}{(E - E_0)^2 + \frac{1}{4}\Gamma^2} \quad \text{.....(1)}$$

where k is the neutron wave number, g_J is a spin statistical weight factor, Γ_n is the neutron width, Γ_γ is the radiative width, Γ is the total width, E_0 is the energy of the resonance and E is the energy. It is assumed that σ is measured in m^2, and E in J. Note that the second fraction is dimensionless and so it can be assumed that all the terms are measured in eV.

The relationship between E and k is shown in equation (2):

$$E = \frac{\hbar^2 k^2}{2m} \quad \text{.....(2)}$$

The energy dependence of Γ_n is shown in equation (3):

$$\Gamma_n = \Gamma_n^0 \sqrt{E} \quad \text{.....(3)}$$

where Γ_n^0 is the reduced neutron width (units of eV are used).

Using the numerical values of all the constants the basic formula can be rewritten so that σ is measured in b, and E in eV. The numerical values are:

$\hbar$ = 1.05457266 10^{-34} Js

m = 1.008664904 u

1 u = 1.6605402 10^{-27} kg

1 J = 6.2415064 10^{18} eV

1 b = 1 10^{-28} m^2

Thus using f as the dimensionless fraction, the basic formula (with units in brackets) is given by equation (4):

$$\sigma(m^2) = \frac{\pi g_J \hbar^2 (Js)}{2m(kg)E(J)} f \quad \text{.....(4)}$$

Using the numerical values equation (4) can be written as equation (5):

$$\sigma(b) = \frac{Cg_J}{E(eV)} f \quad \text{.....(5)}$$

where $C = 6.50977546\ 10^5$

Assuming that all energies that follow are measured in eV and all cross sections in b, and that the non-elastic contribution to the total width can be neglected then equation (1) can be written as equation (6):

$$\sigma = \frac{Cg_J}{\sqrt{E}} \frac{\Gamma_n^0 \Gamma_\gamma}{(E - E_0)^2 + \frac{1}{4}(\Gamma_n + \Gamma_\gamma)^2} \quad \text{.....(6)}$$

In order to determine Γ_n^0 the thermal cross section value is used (and assuming that $E_0 >> E_t$ and $E_0 >> \Gamma$) as shown by equation (7):

$$\sigma_t = \frac{Cg_J}{\sqrt{E_t}} \frac{\Gamma_{n0} \Gamma_\gamma}{E_0^2} \quad \text{.....(7)}$$

In the present version of SAFEPAQ-II the following additional simplifications are used:

- A value of 0.5 is assumed for g_J.
- A simple systematic is used for the radiative width as shown in equation (8) for targets with A < 40:

$$\Gamma_\gamma = 1593 / A^2 \quad \text{.....(8)}$$

where A is the mass number of the target. In cases where A ≥ 40, a table of widths stored in the Parameter database is used.

With these assumptions equation (6) can be used to calculate cross section values from $1\ 10^{-5}$ eV to E_H.

A similar treatment is used for the (n,f) reactions. In this case Γ_γ is replaced by Γ_f. It is assumed by default that $\Gamma_f = 0.235$ eV for fissile targets and $7\ 10^{-4}$ eV for non-fissile targets.

Appendix 6. Low Energy Approximation

It has been demonstrated experimentally [1] that the low energy component of the (n,γ), (n,p) or (n,α) cross sections (for targets with $Q > 0$) have the same energy dependence, namely $1/v$ connected to the resonance region. The similarity in the shapes and distribution of resonances in these three reactions has also been demonstrated experimentally. From this a plausible assumption can be formulated, namely that the partial widths $\Gamma_{\gamma i}$, Γ_{pi} and $\Gamma_{\alpha i}$ obey the same χ^2 - distribution (Porter-Thomas) which results in the similar behaviour of total widths Γ_γ, Γ_p and Γ_α with values close to a constant mean value for each reaction.

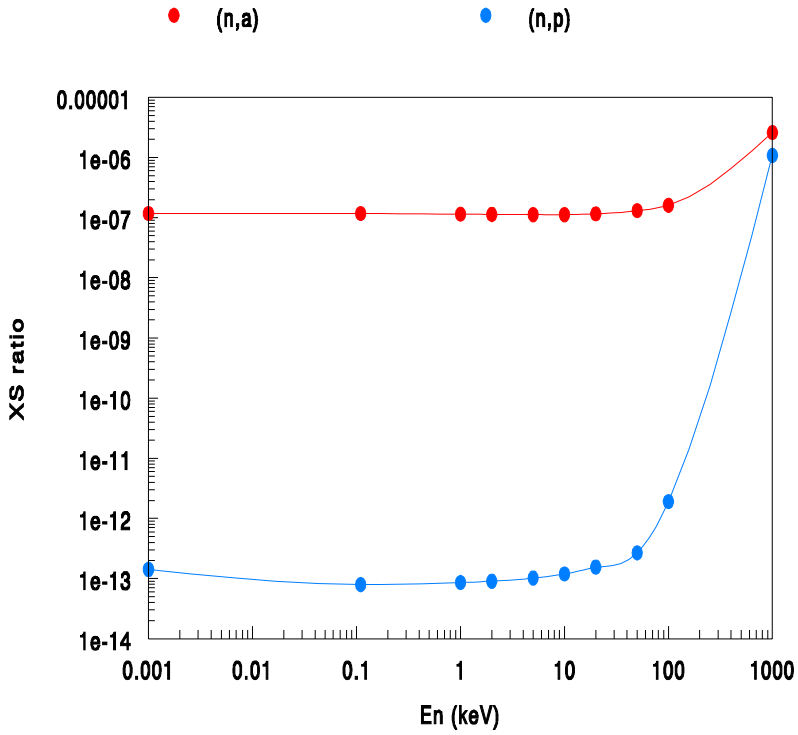


Figure 1. Values of (n,p)/(n,γ) and (n,α)/(n,γ) cross sections for ^{107}Pd and ^{107}Ag targets respectively calculated by TALYS.

These facts have been later supported theoretically by statistical model calculations, which show a constant and energy independent ratio of (n,p)/(n,γ) and (n,α)/(n,γ) cross sections from about 1 meV up to 50-100 keV. This is demonstrated in Figure 1, where the results of calculations with the code TALYS for ^{107}Pd and ^{107}Ag targets are shown. It is obvious that this feature can be used to approximate the unknown low energy component of (n,p) and (n,α) reactions from the known (n,γ) cross sections and smoothly join these data with the excitation curve above the 'effective threshold'. This feature was first used by H. Gruppelaar in 1981 to estimate (n,p)

components in ^{58g}Co and ^{58m}Co evaluations [2] from the total absorption cross section and later in a slight modified version (adjustable MF2 data used to generate data for the resolved resonance region satisfying the thermal (n,p) or (n,α) cross sections) for a small number of reactions on targets in the deformed region between 150 < A < 165 in the JENDL-3 library.

During the development of the TALYS code [3] this idea of the low energy treatment of the non-threshold (n,p) and (n,α) reactions has been included. For normalization of the (n,p) and (n,α) data either the thermal (n,p) and (n,α) cross sections (if experimentally known) or values derived from σ(n,p)/σ(n,γ) or σ(n,α)/σ(n,γ) ratios calculated by TALYS can be used.

This approximation is termed the Low Energy Approximation (LEA), it can be applied to two groups of (n,p) and (n,α) reactions with resolved resonance region in the (n,γ) [MT=102] channel in SAFEPAQ-II.

1. The thermal cross section for the (n,p) or (n,α) reaction is known. In this case the (n,γ) component between 10^{-5} eV and E_H (including the resolved resonance region) is merged with the (n,p) or (n,α) data by means of a Mod type 18 preliminary modification and the low energy (n,γ) component is then normalised to the experimental value of (n,p) or (n,α) thermal cross section.

2. If the thermal cross section for the (n,p) or (n,α) reaction is not known, then the ratio $\sigma^{cal}/\sigma_\gamma^{cal}$ at D_0 is calculated by TALYS and this ratio is used to derive from the known (n,γ) cross section the (n,p) or (n,α) thermal value (σ^{th}) as shown in equation (1).

$$\sigma^{th} = \sigma_\gamma^{th} \times \left(\sigma^{cal} / \sigma_\gamma^{cal}\right) \quad \text{..... (1)}$$

It should be noted, that in both cases the resolved resonance region, if available in the capture reaction, is adopted between 10^{-5} eV and E_H. An illustration of the use of this approximation is shown in Figure 2. The original EAF-2003 data contained a simple 1/*v* component joined to the model calculation at 1 MeV. For TALYS-5a a 1/*v* component is joined to the statistical calculation at 3 keV. In EAF-2005 the resonance data from the ^{39}K(n,γ) reaction is joined to the TALYS-5a data at 300 keV (E_H) to give a improved description of the reaction.

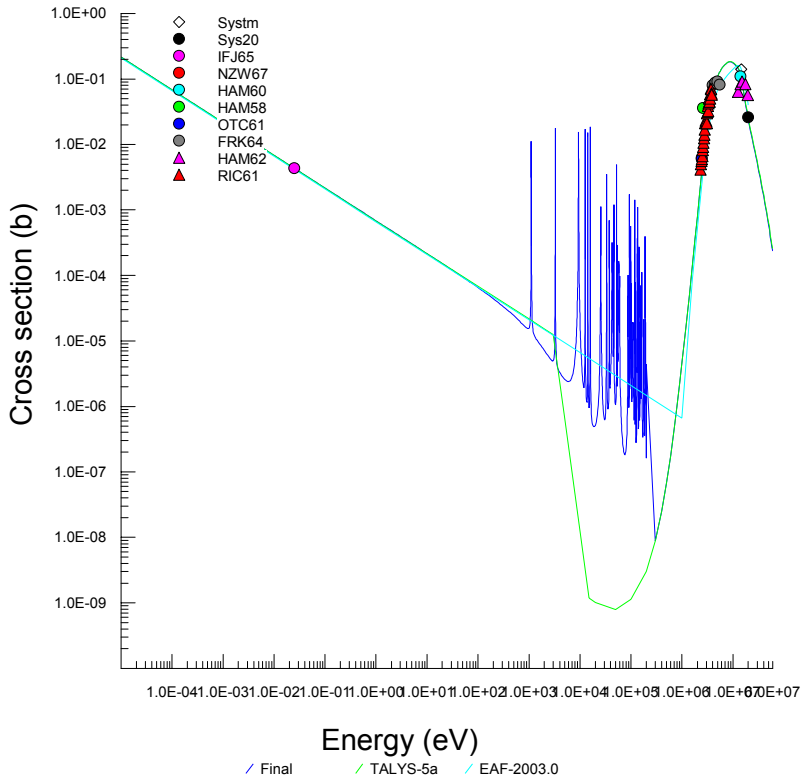


Figure 2. Data for ^{39}K(n,α) in EAF-2003, EAF-2005 (Final) and TALYS-5a.

In cases where no experimental information is available for either the (n,γ) or (n,p), (n,α) reactions, the complete TALYS calculation is adopted. The (n,γ) thermal cross section is estimated from the crude systematic developed in reference 4.

References

[1] Yu. I. Popov and F. L. Shapiro, ZETF, **40**, 1610, 1961.

[2] H. A. J Van der Kamp and H. Gruppelaar, *'Documentation RCN-2 evaluation on ^{58g}Co and ^{58m}Co'*, **FSR-Gr-35** parts 50, 51 (April 1981).

[3] A. J. Koning, S. Hilaire and M. Duijvetsijn, *'TALYS – A nuclear reaction code, User Manual'*, p. 95-97 in Section 4.9, to be published.

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Disclaimer

Neither the authors nor UKAEA accept responsibility for consequences arising from any errors either in the present documentation, the EAF libraries or in the SAFEPAQ-II code.

Contact person

Feedback on the use of EAF and SAFEPAQ-II is welcomed. Please contact R. A. Forrest with comments or in case of problems.

Dr R A Forrest
EURATOM/UKAEA Fusion Association
D3/1.92 Culham Science Centre
Abingdon
Oxfordshire OX14 3DB
Tel: +44 1235 466586
Fax: +44 1235 466435
e-mail: robin.forrest@ukaea.org.uk
Internet: www.fusion.org.uk/easy2007